AN INVESTIGATION OF A NEW CLASS OF LINEAR FINITE DIFFERENCE OPERATORS TO BE USED IN SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

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THESIS

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ABSTRACT

A new technique for constructing "computational molecules" for linear finite difference operators is developed. The basic approach is one of approximating a two dimensional surface with a geometrically consistent interpolating polynomial of degree four or five. The desired finite difference operator is then developed from the polynomial. The resulting molecules are geometrically consistent and may be used to solve boundary value problems without the use of fictitious points.

Molecules for the biharmonic operator with various boundary conditions included are presented in this paper, as well as molecules representing the boundary conditions for shear and moment along the free edge of a plate.

The integrity of the molecules presented is proven by comparison of solutions for flat plate bending problems by finite difference with exact solutions from the literature. Convergence plots for each problem are also presented.

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NOMENCLATURE

$A_{,ab}$	Differentiation of some function A with respect to variables (a) and (b).
C_i	Constants for an interpolating polynomial of degree four.
D	Flexural rigidity: $\frac{E\tau^3}{12(1-\mu^2)}$
D_i	Constants for an interpolating polynomial of degree.
E	Young's modulus of elasticity.
E_t	Error of approximation.
$F^{(i)}(x,y)$	Expression for variable terms of an interpolating polynomial of degree four.
$G^{(i)}(x,y)$	Expression for variable terms of an interpolating polynomial of degree five.
h	Mesh size spacing.
L	Length or width.
M_n	Moment in the normal direction along the edge of a flat plate.
N	Number of divisions on one side of a square finite difference mesh.
n	Normal co-ordinate.
p	Applied pressure
P(x,y)	Interpolating polynomial.
P_i	Values of polynomial at various nodal points.
t	Tangential co-ordinate.
V	Transverse shear along a free edge of a plate.
x	Horizontal co-ordinate.
y	Vertical co-ordinate
δ	Plate deflection.
μ	Poisson's ratio

$\{\ \}$	Matrix notation for column vector.
$\langle\ \rangle$	Matrix notation for row vector.
$[\ ]$	Square or rectangular matrix.
∇^2	Harmonic operator.
∇^4	Biharmonic operator.
τ	Thickness of a thin plate.
$\mathcal{O}$	Order of

I. INTRODUCTION

A. GENERAL DESCRIPTION

Solving partial differential equations and boundary value problems by approximate numerical methods is not new. Such numerical solutions have become very popular in the past twenty years due to the development of the high speed digital computer.

One widely used numerical method for solving partial differential equations is that of finite differences. The solution of equations by this method leads to the development of "computational molecules". Various techniques have been used to develope such molecules and numerous molecules are available in the literature (Refs. 1,2,3,&4).

Often these molecules tend to be geometrically inconsistent. This inconsistency results from combining molecules for the elementary differential operators, developed from different interpolating polynomials, in order to obtain a more complex operator. For instance, the molecule for the biharmonic operator as given by Salvadori and Baron (Ref. 1) utilizes two different interpolating formulas. The fourth derivatives are obtained from a polynomial of degree four. The mixed partial derivative is obtained from a bi-quadratic interpolating surface.

Furthermore, the application of these molecules in the solution of boundary value problems requires the use of fictitious nodal points outside the physical boundaries of the problem. Relationships between these fictitious nodal points and those nodal points representing the physical problem must be pre-determined. When the fictitious points cannot be determined uniquely, the method fails.

Considering the above disadvantages of the classical finite difference operators found in the literature, the objective of the author's research was to develope a new technique for constructing linear finite difference operators. This new technique utilizes one consistent form of an interpolating polynomial to approximate a two dimensional surface from which molecules for all operators are constructed. Furthermore, basic operators incorporating physical boundary conditions are constructed using this technique. The use of such operators alleviates the need for fictitious nodal points.

The technique proposed in this research is applicable for the construction of any finite difference operator. However, the field of investigation for the purpose of this research was limited to the construction of those operators required for the solution of plate bending problems with various boundary conditions. The solutions of such problems will be used to justify the integrity of the constructed finite difference operators.

B. BASIC TECHNIQUE

The basic technique employed to construct the molecules for a prescribed linear finite difference operator is one of approximating a two dimensional surface by means of a biquadratic or biquintic interpolating polynomial. The constants for such an interpolating polynomial are determined for each desired surface, which may include specified boundary conditions, using a finite difference grid. The polynomial is

then operated on with the desired partial differential operator to be approximated.

The final result is a numerical approximation of the operator in terms of a computational molecule, grid size, nodal deflections, and nodal boundary condition values.

All calculations required for the construction of these molecules were performed in double precision using an IBM-360 computer.

II. DERIVATION OF DIFFERENTIAL OPERATORS

A. INTERPOLATING POLYNOMIALS

The interpolating polynomials used to approximate a two dimensional surface for the development of a finite difference biharmonic operator in this work were either

$$\begin{aligned} P(x,y) = \; & C_1y^4x^4+ C_2y^3x^4+ C_3y^2x^4+ C_4yx^4+ C_5x^4 \\ & + C_6y^4x^3+ C_7y^3x^3+ C_8y^2x^3+ C_9yx^3+C_{10}x^3 \\ & +C_{11}y^4x^2+C_{12}y^3x^2+C_{13}y^2x^2+C_{14}yx^2+C_{15}x^2 \\ & +C_{16}y^4x +C_{17}y^3x +C_{18}y^2x +C_{19}yx +C_{20}x \\ & +C_{21}y^4 +C_{22}y^3 +C_{23}y^2 +C_{24}y +C_{25} \end{aligned} \tag{2.1}$$

and in matrix notation

$$P(x,y) = \langle F^{(i)}(x,y) \rangle \{C_i\}_{i=1,2,\ldots,25} \tag{2.1a}$$

or

$$\begin{aligned} P(x,y) = \; & D_1y^5x^5+ D_2y^4x^5+ D_3y^3x^5+ D_4y^2x^5+ D_5yx^5+ D_6x^5 \\ & + D_7y^5x^4+ D_8y^4x^4+ D_9y^3x^4+D_{10}y^2x^4+D_{11}yx^4+D_{12}x^4 \\ & +D_{13}y^5x^3+D_{14}y^4x^3+D_{15}y^3x^3+D_{16}y^2x^3+D_{17}yx^3+D_{18}x^3 \\ & +D_{19}y^5x^2+D_{20}y^4x^2+D_{21}y^3x^2+D_{22}y^2x^2+D_{23}yx^2+D_{24}x^2 \\ & +D_{25}y^5x +D_{26}y^4x +D_{27}y^3x +D_{28}y^2x +D_{29}yx +D_{30}x \\ & +D_{31}y^5 +D_{32}y^4 +D_{33}y^3 +D_{34}y^2 +D_{35}y +D_{36} \end{aligned} \tag{2.2}$$

and in matrix notation

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \quad \{D_i\}_{i=1,2,\ldots,36} \qquad (2.2a)$$

Polynomials (2.1) (2.2) will remain polynomials of degree four or five respectively for both constant values of x and y. All partial derivatives with respect to x and y of order four exist. Either polynomial will consistently approximate a two dimensional surface.

In certain cases, a fifth order polynomial such as (2.2) which will approximate a thirty-six nodal point grid surface is required in the construction of the biharmonic operator molecule with included boundary conditions. This requirement results from the need for keeping the error of approximation for a given molecule of an order equal to or greater than the square of the grid size spacing. The subject of approximation error will be further discussed later.

B. BASIC FINITE DIFFERENCE BIHARMONIC OPERATOR

For the solution of a problem governed by a partial differential equation, in which the biharmonic operator appears, a numerical approximation of the biharmonic operator without boundary conditions must be constructed first. To construct the molecule for such an operator polynomial (2.1) was used to approximate a two dimensional surface defined by the ordinates at the nodes of a grid shown in Figure (1).

To determine the unknown constants for the interpolating polynomial, the polynomial was evaluated at each of the

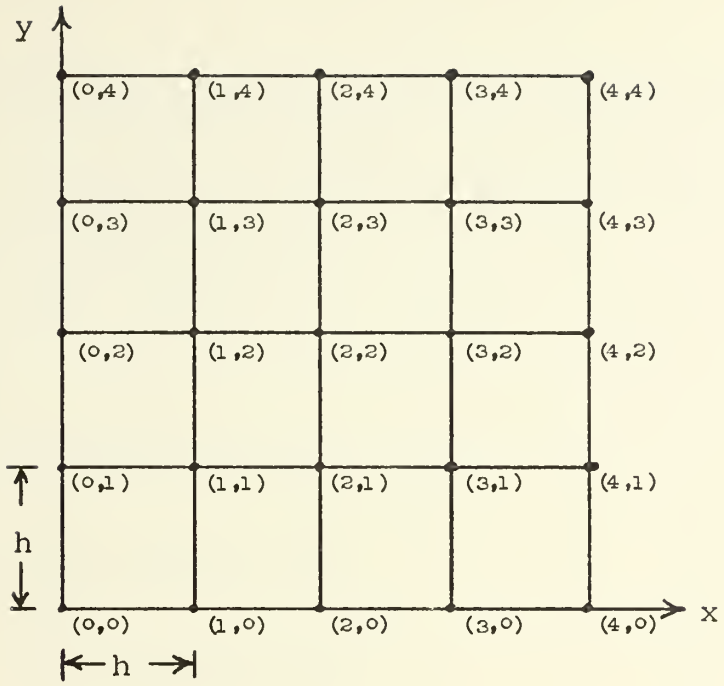

Figure 1 - 5 x 5 Equally Spaced Grid

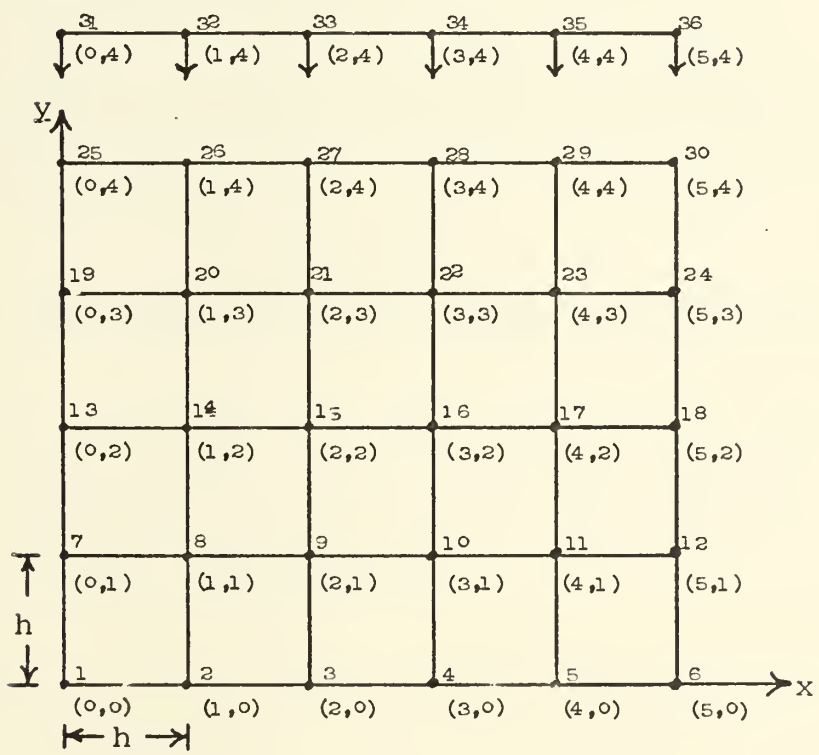

Figure 2 - 5 x 6 Equally Spaced Grid With The Top Edge Repeated

twenty-five nodal points in terms of the co-ordinate values of x and y. In matrix notation, the resulting system of equations are expressed as

$$\{P_i\} = [M] \{C_i\}_{i=1,2,\ldots,25} \tag{2.3}$$

where

$$\{P_i\} = \{P(x_i,y_i)\}_{i=1,2,\ldots,25}$$

$$[M] = \begin{bmatrix} \langle F^{(i)}(x_1,y_1) \rangle \\ \langle F^{(i)}(x_2,y_2) \rangle \\ \vdots \\ \langle F^{(i)}(x_{25},y_{25}) \rangle \end{bmatrix}_{i=1,2,\ldots,25}$$

Solving equation (2.3) for the unknown coefficients, yields

$$\{C_i\} = [M]^{-1} \{P_i\}_{i=1,2,\ldots,25} \tag{2.4}$$

with which the interpolating polynomial is rewritten as

$$P(x,y) = \langle F^{(i)}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,\ldots,25} \tag{2.5}$$

Operating on equation (2.5) with the biharmonic operator results in the following equation

$$\nabla^4 P(x,y) = \langle \nabla^4 F^{(i)}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,\ldots,25} \tag{2.6}$$

The quantity $\langle \nabla^4 F^{(i)}(x,y) \rangle$ is now evaluated for a particular nodal point say m(x=2h,y=2h). The resulting quantity

$\langle \nabla^4 F^{(i)}(2h,2h) \rangle [M]^{-1}$ after numerical evaluation yields a five by five computational molecule for the finite difference biharmonic operator at nodal point (m).

The above molecule allows for the numerical approximation of the biharmonic operator in terms of known constants and nodal deflections. Evaluation of a computational molecule for a nodal point other than the center one is performed in a similar manner except that polynomial (2.2) and a six by six grid is used in order to achieve an acceptable bound on the error of approximation.

C. FINITE DIFFERENCE BIHARMONIC OPERATORS WITH BOUNDARY CONDITIONS SPECIFIED

To complete the solution of a boundary value problem, the applicable boundary conditions must be considered. If geometric considerations alone are required for the boundary conditions, a general finite difference molecule for the biharmonic operator incorporating the desired boundary conditions may be developed. The technique uses polynomial (2.2) to approximate a surface having the desired boundary conditions.

1. Operators With First Partial Derivative Boundary Conditions

For the construction of a finite difference biharmonic operator with a first partial with respect to y boundary condition, polynomial (2.2) is used to approximate a surface such as the one represented by Figure (2) where the nodal points along the top edge are repeated to accommodate both

values of deflection and the specified boundary conditions along that edge.

The unknown coefficients for the interpolating polynomial are determined by evaluating the polynomial at each of the thirty distinct nodal points and the first partial with respect to y of the polynomial at each of the nodal points along the top edge. The resulting equations are

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.7}$$

$$P_{,y}(x,y) = \langle G^{(i)}_{,y}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.8}$$

The complete system of equations becomes

$$\{P_i\} = [M_1] \{D_i\}_{i=1,2,\ldots,36} \tag{2.9}$$

where

$$\{P_i\} = \langle P(x_j,y_j) \mid P_{,y}(x_k,y_k) \rangle^T$$

$$[M_1] = \begin{bmatrix} \langle G^{(i)}(x_j,y_j) \rangle_{j=1,2,\ldots,30} \\ \vdots \\ \hline \langle G^{(i)}_{,y}(x_k,y_k) \rangle_{k=31,32,\ldots,36} \end{bmatrix}_{i=1,2,\ldots,36}$$

and solving for the unknown coefficients

$$\{D_i\} = [M_1]^{-1} \{P_i\}_{i=1,2,\ldots,36} \tag{2.10}$$

from which the interpolating polynomial may be written as

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \quad [M_1]^{-1} \{P_i\}_{i=1,2,\ldots,36} \qquad (2.11)$$

Operating on equation (2.11) with the biharmonic operator results in the following equation

$$\nabla^4 P(x,y) = \langle \nabla^4 G^{(i)}(x,y) \rangle \quad [M_1]^{-1} \{P_i\}_{i=1,2,\ldots,36} \qquad (2.12)$$

The quantity $\langle \nabla^4 G^{(i)}(x,y) \rangle$ is evaluated for any desired nodal point within the grid and the resulting numerical evaluation of $\langle \nabla^4 G^{(i)}(x,y) \rangle \quad [M_1]^{-1}$ gives a six by six molecule for the biharmonic operator with the prescribed boundary conditions.

For first partial derivatives with respect to x and to y along two perpendicular edges, the respective biharmonic molecule is developed using polynomial (2.2) to approximate the surface defined by ordinates at the nodes of the grid given in Figure (3). The nodal points along two perpendicular edges are repeated to account for both the values of deflections and the boundary conditions at these nodal points.

The coefficients for the interpolating polynomial are determined from the following relationships

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \quad \{D_i\}_{i=1,2,\ldots,36} \qquad (2.13)$$

$$P_{,y}(x,y) = \langle G^{(i)}_{,y}(x,y) \rangle \quad \{D_i\}_{i=1,2,\ldots,36} \qquad (2.14)$$

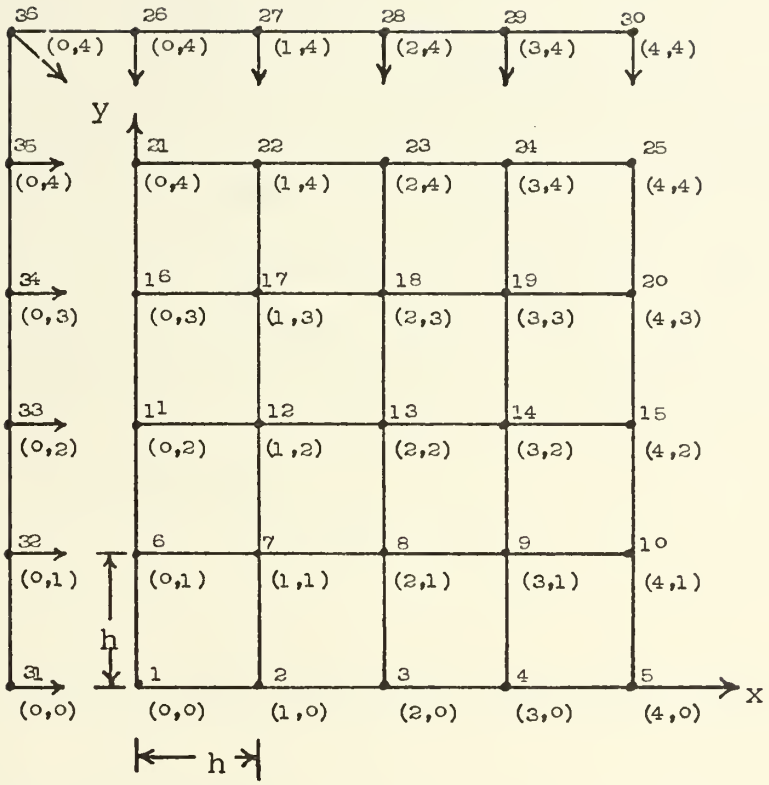

Figure 3 - 5 x 5 Equally Spaced Grid With Two Perpendicular Edges Repeated

$$P_{,x}(x,y) = \langle G^{(i)}_{,x}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.15}$$

$$P_{,xy}(x,y) = \langle G^{(i)}_{,xy}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.16}$$

The mixed second partial was used in the development in order to have sufficient conditions to evaluate the thirty six coefficients of the interpolating polynomial and to provide for continuity at the common corner nodal point.

The complete system of equations becomes

$$\{P_i\} = [M_2] \{D_i\}_{i=1,2,\ldots,36} \tag{2.17}$$

where

$$\{P_i\} = \langle P(x_j,y_j) \mid P_{,y}(x_k,y_k) \mid P_{,x}(x_\ell,y_\ell) \mid P_{,xy}(x_m,y_m) \rangle^T$$

$$[M_2] = \begin{bmatrix} \langle G^{(i)}(x_j,y_j) \rangle_{j=1,2,\ldots,25} \\ \vdots \\ \hline \langle G^{(i)}_{,y}(x_k,y_k) \rangle_{k=26,27,\ldots,30} \\ \vdots \\ \hline \langle G^{(i)}_{,x}(x_\ell,y_\ell) \rangle_{\ell=31,32,\ldots,35} \\ \vdots \\ \hline \langle G^{(i)}_{,xy}(x_m,y_m) \rangle_{m=36} \end{bmatrix}_{i=1,2,\ldots,36}$$

Solving for the constants, $\{D_i\}$, and operating on the resulting polynomial with the biharmonic operator yields

$$\nabla^4 P(x,y) = \langle \nabla^4 G^{(i)}(x,y) \rangle \; [M_2]^{-1} \; \{P_i\}_{i=1,2,\ldots,36} \qquad (2.18)$$

where $\langle \nabla^4 G^{(i)}(x,y) \rangle \; [M_2]^{-1}$ is evaluated for any desired nodal point. The result is a molecule for the biharmonic operator with the desired specified boundary conditions.

2. Operators With Second Partial Derivative Boundary Conditions

A biharmonic operator for a region with the harmonic operator specified along a part of the boundary is often required for the solution of a boundary value problem. The required molecule for the biharmonic operator with such specified boundary conditions is developed using polynomial (2.2) and the grid of Figure (2). The applicable equations for determining the constants of the polynomial are

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.19)$$

$$\nabla^2 P(x,y) = \langle \nabla^2 G^{(i)}(x,y) \rangle \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.20)$$

from which the system of equations becomes

$$\{P_i\} = [M_3] \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.21)$$

where

$$\{P_i\} = \langle P(x_j,y_j) \,|\, \nabla^2 P(x_k,y_k) \rangle^T$$

$$[M_3] = \begin{bmatrix} \langle G^{(i)}(x_j,y_j) \rangle_{j=1,2,\ldots,30} \\ \vdots \\ \hline \langle \nabla^2 G^{(i)}(x_k,y_k) \rangle_{k=31,32,\ldots,36} \end{bmatrix}_{i=1,2,\ldots,36}$$

Solving for the unknown constants and operating on the resulting polynomial with the biharmonic operator yields the desired relationship for determining the biharmonic molecule. The relationship for the operator with the specified boundary condition is

$$\nabla^4 P(x,y) = \langle \nabla^4 G^{(i)}(x,y) \rangle \; [M_3]^{-1} \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.22)$$

For boundary conditions requiring the second partial with respect to y along one edge and the second partial with respect to x along a perpendicular edge, polynomial (2.2) and the grid of Figure (3) is used in the development of the applicable biharmonic molecule. The equations required to determine the appropriate constants for the interpolating polynomial are

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.23)$$

$$P_{,yy}(x,y) = \langle G^{(i)}_{,yy}(x,y) \rangle \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.24)$$

$$P_{,xx}(x,y) = \langle G^{(i)}_{,xx}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \quad (2.25)$$

$$\nabla^2 P(x,y) = \langle \nabla^2 G^{(i)}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \quad (2.26)$$

$$P_{,xxy}(x,y) = \langle G^{(i)}_{,xxy}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \quad (2.27)$$

$$P_{,yyx}(x,y) = \langle G^{(i)}_{,yyx}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \quad (2.28)$$

Conditions expressed by equations (2.26), (2.27), and (2.28) are required to obtain sufficient independent equations with which to determine the thirty-six unknown constants. The values for these additional nodal boundary conditions are handled as additional unknowns. The resulting set of equations for determining the unknown constants of the required polynomial is

$$\{P_i\} = [M_4] \{D_i\}_{i=1,2,\ldots,36} \quad (2.29)$$

where

$$\{P_i\} = \langle P(x_j,y_j) \mid P_{,yy}(x_k,y_k) \mid P_{,xx}(x_\ell,y_\ell) \mid$$

$$\nabla^2 P(x_{26},y_{26}), P_{,xxy}(x_{35},y_{35}), P_{,yyx}(x_{36},y_{36}) \rangle^T$$

$$[M_4] = \begin{bmatrix} \langle G^{(i)}(x_j,y_j) \rangle \\ \vdots \\ \hline \langle G^{(i)}_{,yy}(x_k,y_k) \rangle \\ \vdots \\ \hline \langle G^{(i)}_{,xx}(x_\ell,y_\ell) \rangle \\ \vdots \\ \hline \langle \nabla^2 G^{(i)}(x_{26},y_{26}) \rangle \\ \\ \langle G^{(i)}_{,xxy}(x_{35},y_{35}) \rangle \\ \\ \langle G^{(i)}_{,yyx}(x_{36},y_{36}) \rangle \end{bmatrix}_{\substack{j=1,2,\ldots,25 \\ k=29,28,\ldots,30 \\ \ell=31,32,\ldots,34 \\ i=1,2,\ldots,36}}$$

(a)

The final form of the desired finite difference biharmonic operator is

$$\nabla^4 P(x,y) = \langle \nabla^4 G^{(i)}(x,y) \rangle \; [M_4]^{-1} \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.30)$$

3. Operators With Mixed Boundary Conditions

The development of a biharmonic molecule with boundary conditions of the first partial with respect to y along one edge

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(a) It should be noted that points 26, 35, and 36 all have the same geometrical co-ordinates.

and the harmonic condition along a perpendicular edge utilizes interpolating polynomial (2.2) and the grid of Figure (3). The applicable equations for determining the required constants for the interpolating polynomial are

$$P(x,y) = \langle G^{(i)}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.31}$$

$$P_{,y}(x,y) = \langle G^{(i)}_{,y}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.32}$$

$$\nabla^2 P(x,y) = \langle \nabla^2 G^{(i)}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.33}$$

$$P_{,xy}(x,y) = \langle G^{(i)}_{,xy}(x,y) \rangle \{D_i\}_{i=1,2,\ldots,36} \tag{2.34}$$

The resulting system of equations is

$$\{P_i\} = [M_5] \{D_i\}_{i=1,2,\ldots,36} \tag{2.35}$$

where

$$\{P_i\} = \langle P(x_j,y_j) \mid P_{,y}(x_k,y_k) \mid \nabla^2 P(x_\ell,y_\ell) \mid P_{,xy}(x_{36},y_{36}) \rangle^T$$

$$[M_5] = \begin{bmatrix} \langle G^{(i)}(x_j,y_j) \rangle \\ \vdots \\ \hline \langle G^{(i)}_{,y}(x_k,y_k) \rangle \\ \vdots \\ \hline \langle \nabla^2 G^{(i)}(x_\ell,y_\ell) \rangle \\ \vdots \\ \hline \langle G^{(i)}_{,xy}(x_{36},y_{36}) \rangle \end{bmatrix}_{i=1,2,\ldots,36}$$

$j=1,2,\ldots,25$; $k=26,27,\ldots,30$; $\ell=31,32,\ldots,35$

The final form of the desired finite difference biharmonic operator is

$$\nabla^4 P(x,y) = \langle \nabla^4 G^{(i)}(x,y) \rangle \; [M_5]^{-1} \; \{D_i\}_{i=1,2,\ldots,36} \qquad (2.36)$$

4. Other Finite Difference Operators

Certain physical boundary conditions include values of material properties in their evaluations. For example, in plate bending two such conditions are the equations for the moment and the shear along the free edge of a flat plate under some loading. The technique of combining the biharmonic operator and such boundary conditions into a single finite difference molecule is not practical in such cases. The reason being that in order to invert the matrices encountered in the development of the desired molecule, the material property

would have to be specified before the inversion of matrix [M]. This would limit the application of the molecule to a specific material.

To prevent this limitation, a molecule for the desired boundary condition alone is developed using the consistent interpolating polynomial (2.1). The technique is one of developing individual molecules for the partial derivatives involved in the boundary condition. The individual molecules are then combined with the applicable physical properties to form a general molecule which will represent the boundary condition.

An example of this approach is illustrated in the development of molecules for the moment and the shear along the free edge of a flat plate. The governing equations are (Ref. 5)

$$M_n = D(P_{,nn}(x,y) + \mu P_{,tt}(x,y)) = 0 \qquad (2.37)$$

and

$$V = D(P_{,nnn}(x,y) + (2-\mu) P_{,ntt}(x,y)) = 0 \qquad (2.38)$$

where n is the normal co-ordinate, t the tangential co-ordinate, and μ is Poisson's ratio and D the flexural rigidity of the plate.

Molecules for each of the derivatives in equations (2.37) and (2.38) are developed by using the interpolating polynomial in the form given by (2.5). Operating on the interpolating polynomial with the required differential operators yields the following relationships

$$P_{,nn}(x,y) = \langle F^{(i)}_{,nn}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,...,25} \quad (2.39)$$

$$P_{,tt}(x,y) = \langle F^{(i)}_{,tt}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,...,25} \quad (2.40)$$

$$P_{,nnn}(x,y) = \langle F^{(i)}_{,nnn}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,...,25} \quad (2.41)$$

$$P_{,ttn}(x,y) = \langle F^{(i)}_{,ttn}(x,y) \rangle \quad [M]^{-1} \{P_i\}_{i=1,2,...25} \quad (2.42)$$

Evaluation of the above relationships at a nodal point along the boundary of the grid given in Figure (1) yields the required molecule for each derivative.

The molecules are then combined to form the following finite difference approximations for equations (2.37) and (2.38).

$$M_n = D(\langle F^{(i)}_{,nn}(x,y) \rangle \quad [M]^{-1} + \mu \quad \langle F^{(i)}_{,tt}(x,y) \rangle \quad [M]^{-1}) \{P_i\} \quad (2.43)$$

$$V = D(\langle F^{(i)}_{,nnn}(x,y) \rangle \quad [m]^{-1} + (2-\mu) \quad \langle F^{(i)}_{,ttn}(x,y) \rangle \quad [M]^{-1} \{P_i\} \quad (2.44)$$

D. ERROR OF APPROXIMATION

The molecules developed in this work are based on approximating a two dimensional surface with a polynomial. Before the results can be effectively used, a bound on the error entailed in this approximation is essential.

The error of approximation for a finite difference biharmonic operator for some nodal point (m) is defined as

$$E_t = \frac{\partial^4 P_m}{\partial x^4} + 2 \frac{\partial^4 P_m}{\partial x^2 \partial y^2} + \frac{\partial^4 P_m}{\partial y^4} - \nabla^4 P_m(x,y)_{(APPROX.)} \qquad (2.45)$$

The approximate value of the biharmonic operator at nodal point (m) is determined from the appropriate computational molecule and the nodal values associated with the molecule.

An evaluation of the required nodal values appearing in the approximate operator, can be obtained from a Taylor Series Expansion in two variables. If a Taylor Series Expansion is centered on nodal point (m), values for all other nodal points in the grid may be expressed in terms of the nodal value at (m), its partial derivatives, and the grid spacing. Values for the nodal derivatives specified by the boundary conditions are also expressed in terms of the nodal point (m) by using the respective derivatives of the Taylor Series Expansion.

Consequent evaluation of the required nodal values in terms of nodal point (m) and substitution into relationship (2.45) yields the following relationship for the error of approximation

$$E_t = \sum_{i=1}^{\infty} E_i \, h^{n_i} \frac{\partial^{n_i+4} P_m}{\partial x^{c_i} \partial y^{(n_i+4-c_i)}} \qquad (2.46)$$

$$n_i = 2,3,\ldots,\infty$$

$$c_i = 6,7,\ldots,\infty$$

$$E_i = \text{CONSTANT}$$

For the purpose of this work the above series was truncated after the first non-zero term in order to obtain a bound on the error for the respective approximate biharmonic operator. After truncation, the error for all of the approximate biharmonic operators developed in this work was found to be proportional to at least the square of the mesh size (h) and a sixth partial derivative with respect to x and y.

With the error proportional to at least the square of the mesh size (h) used for the finite difference approximation, resulting solutions should rapidly converge to the true solution as the finite difference mesh is refined. The true solution should be obtained as the mesh size tends toward zero.

To obtain an error proportional to at least the square of the mesh size spacing in all cases required the use of polynomial (2.2) for the development of all biharmonic molecules with boundary conditions included.

III. RESULTS

The molecules for the various finite difference operators developed by the author in this work are presented in Tables (1) through (8).

Table (1) represents the molecule for the general biharmonic operator evaluated for the center nodal point. This molecule is applicable for all nodal points in a mesh which are at least two nodal points removed from all boundaries.

Table (2) represents the molecules for nodal points (1, 3) and (2,3) to be used to evaluate the biharmonic operator when boundary conditions specify the first partial with respect to y along an edge. Such a case would be the solution of a flat plate bending problem with a built-in edge restraint.

Table (3) represents the molecules for nodal points (1,3), (2,3), and (1,2) to be used to evaluate the biharmonic operator when boundary conditions specify the first partial along two mutual perpendicular edges. Such a case might be the solution for the deflection of a flat plate under uniform pressure with all edges built-in.

Table (4) represents the molecules for nodal points (1,3) and (2,3) to be used for the biharmonic operator when boundary conditions specified by the harmonic operator are required. Such a boundary condition might be the moment for a flat plate with an edge simply supported.

Table (5) represents the molecules for nodal points (1,3), (2,3), and (1,2) to be used to numerically evaluate the biharmonic operator when boundary conditions specify the second

partial with respect to x along one edge of a boundary and the second partial with respect to y along another edge. Such a condition would exist in solving a plate bending problem when all edges are simply supported.

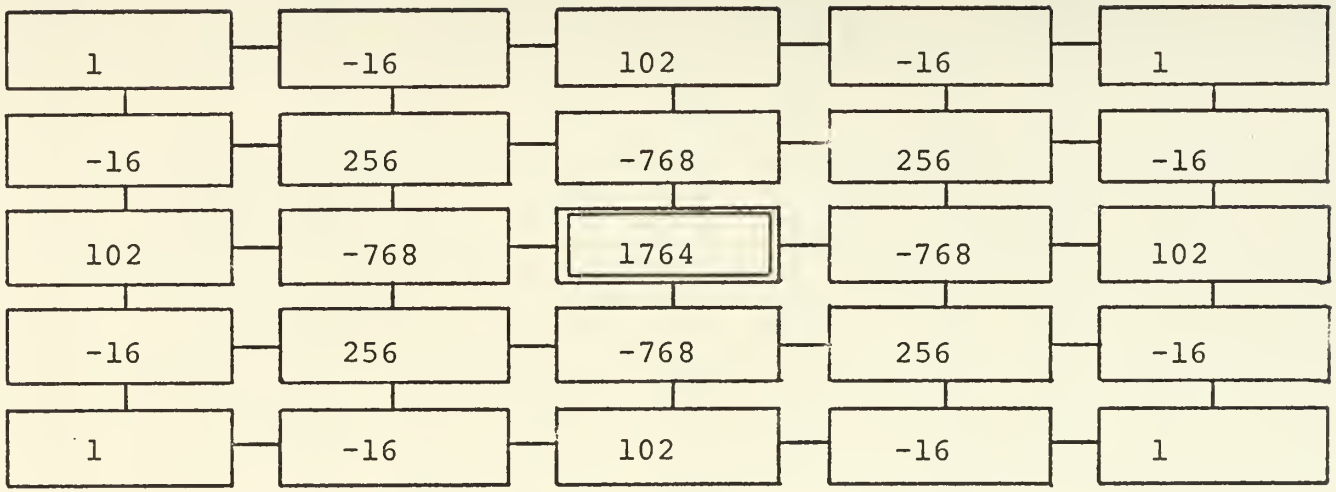
Table (6) represents the molecules for nodal points (1,3), (2,3), and (1,2) to be used to evaluate the biharmonic operator when boundary conditions specify the first partial with respect to y along one boundary and the harmonic operator along an adjacent boundary. Such a case would be for a flat plate with one edge built-in and an adjacent edge simply supported.

Tables (7) and (8) represent the molecules for nodal points (1,0) and (2,0) to be used to numerically evaluate the boundary conditions governed by equations (2.37) and (2.38).

Below each molecule a common factor is given by which the tabulated entries of the molecule must be multiplied. This common factor was generated by converting the original computational values which were in terms of repeating decimal fractions to rational fractions.

Each molecule is presented in a form similar to the grid (Figures 1, 2, and 3) from which it was developed. Consequently each constant in a molecule applies to the respective nodal deflection or boundary condition value in the grid for which it was developed.

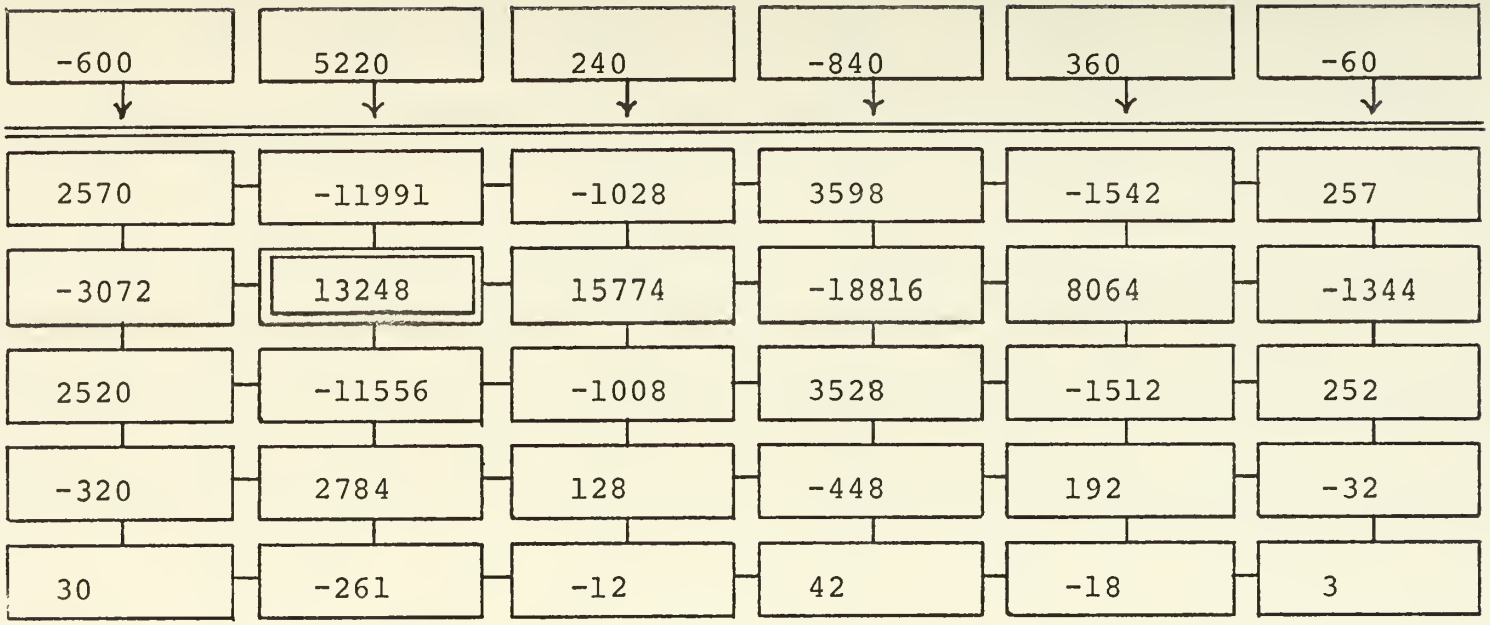
An estimate of the error of approximation is given below each molecule.



Common Factor = $\frac{1}{72h^4}$

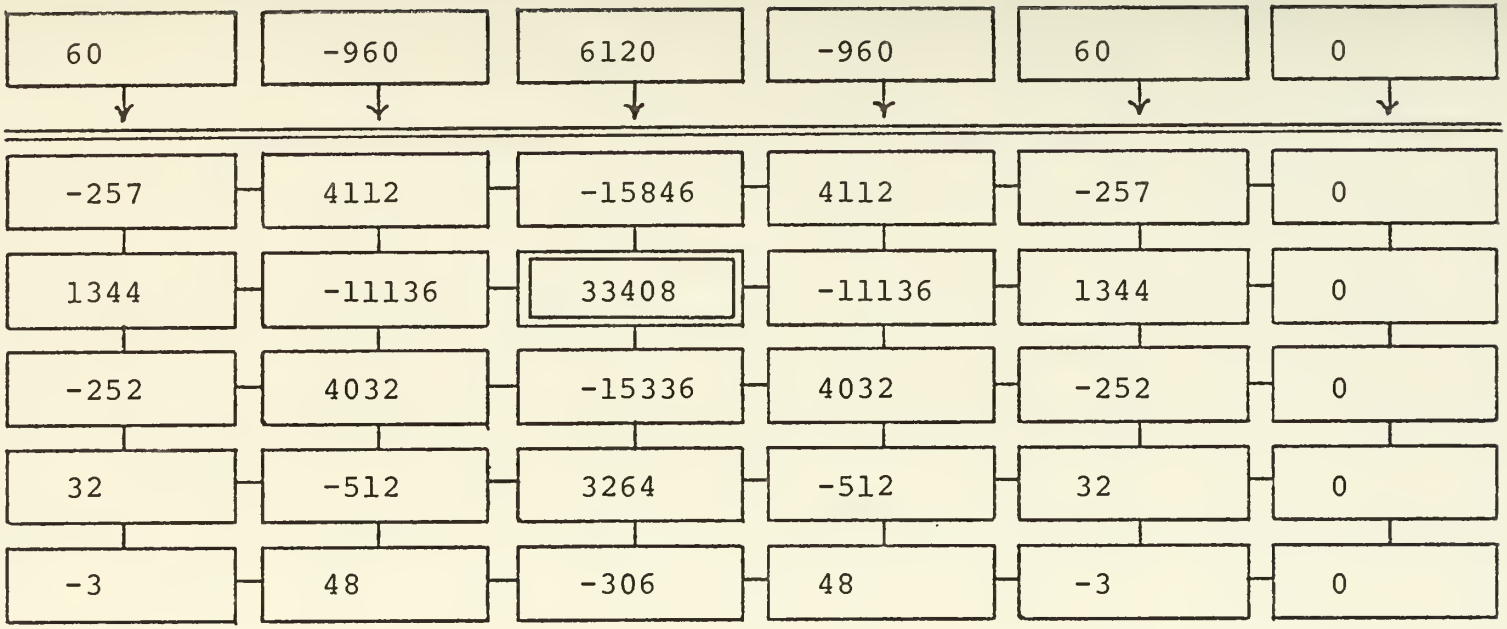
$$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{1}{6} h^2 \frac{\partial^6 P}{\partial y^6}$$

Table 1 - General Biharmonic Operator Molecule



$$\text{Common Factor} = \frac{1}{864h^4} \qquad E_t = \frac{5h^2}{6} \frac{\partial^6 p}{\partial x^6}$$

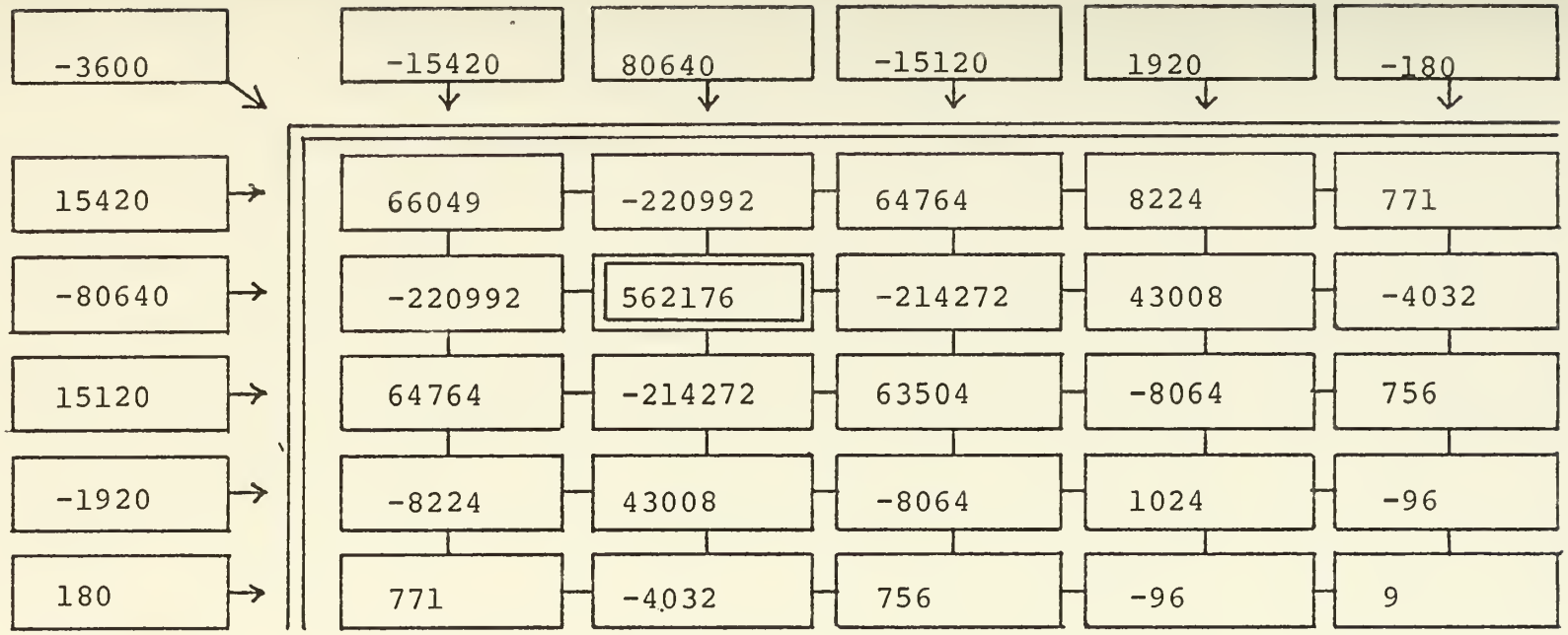
Table 2 - Finite Difference Molecule For Biharmonic Operator With Boundary Condition of $\partial/\partial y$ Along the Top Edge.



Common Factor = $\frac{1}{864h^4}$

$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial x^6}$

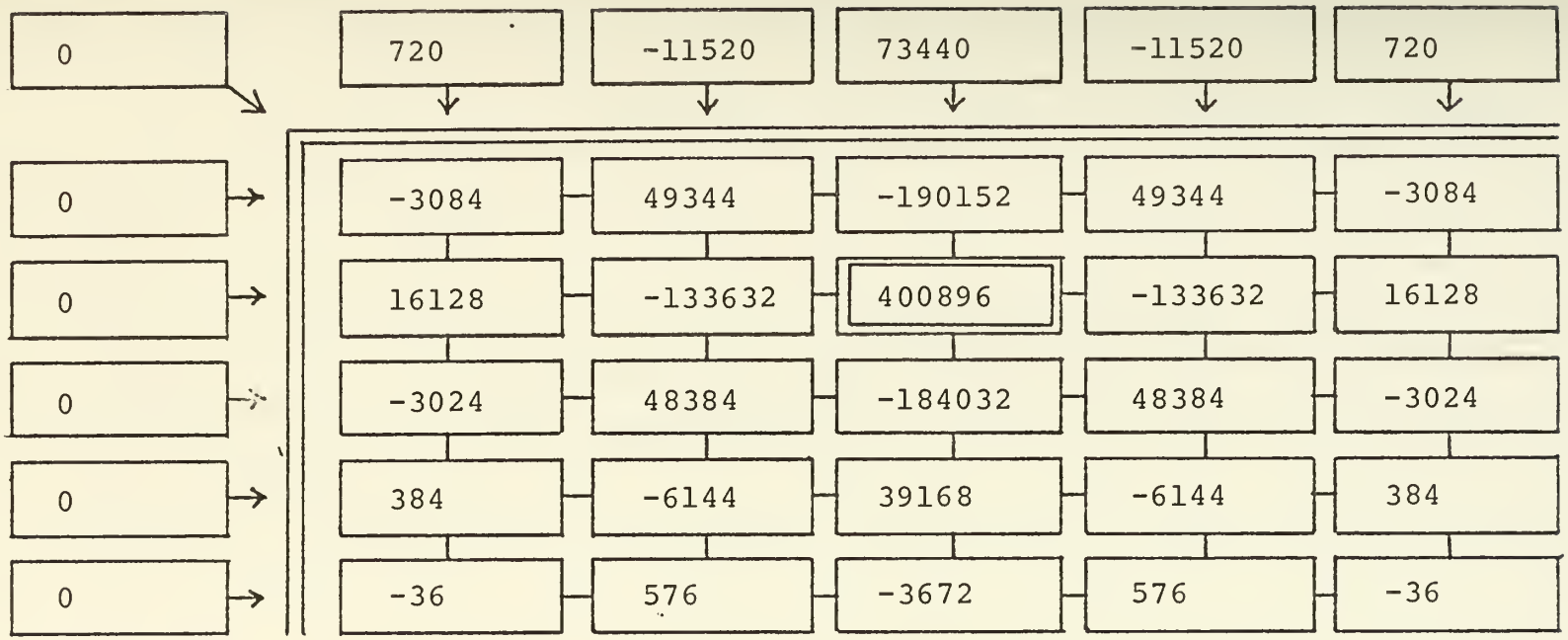
Table 2 - (Continued)



$$\text{Common Factor} = \frac{1}{10,368h^4}$$

$$E_t = +\frac{1}{21} h^3 \frac{\partial^7 P}{\partial x^7} - \frac{1}{21} h^3 \frac{\partial^7 P}{\partial y^7}$$

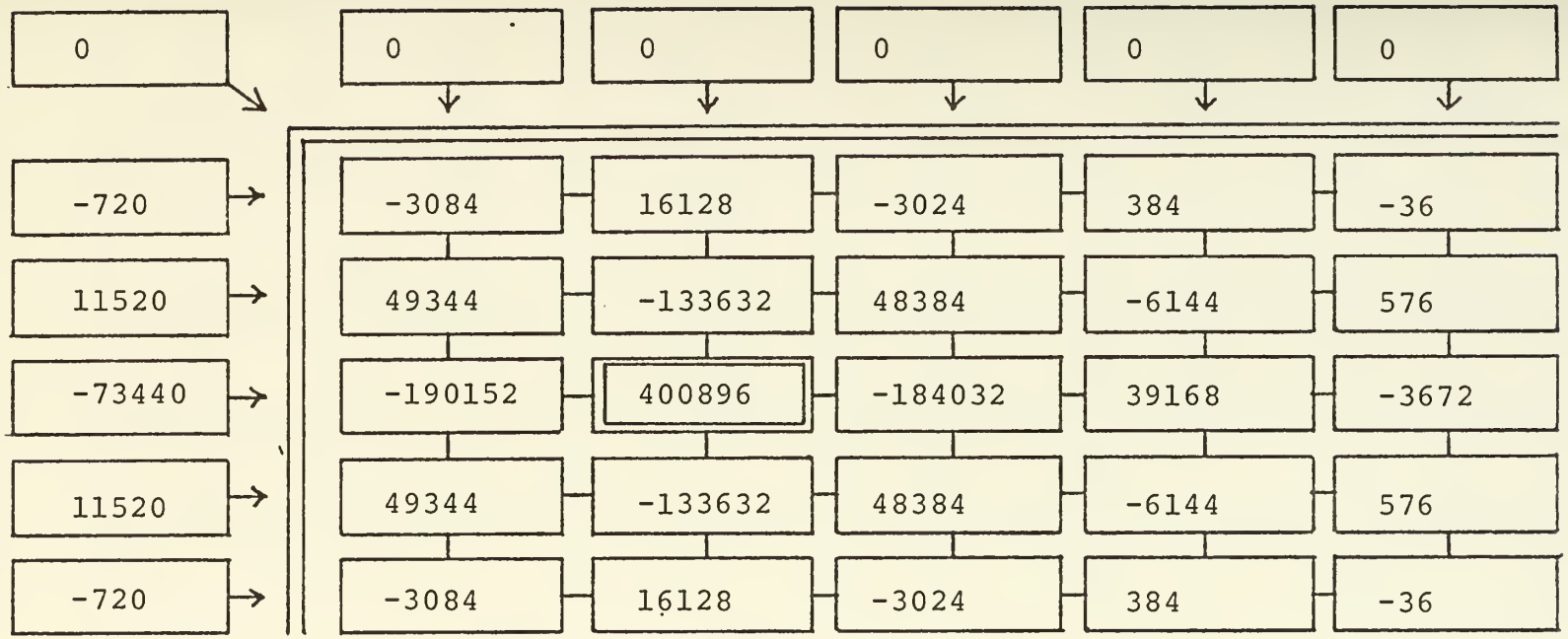
Table 3 - Finite Difference Molecule For Biharmonic Operator With Boundary Conditions of $\partial/\partial y$ Along the Top Edge And $\partial/\partial x$ Along the Left Edge



Common Factor = $\frac{1}{10368h^4}$

$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial x^6}$

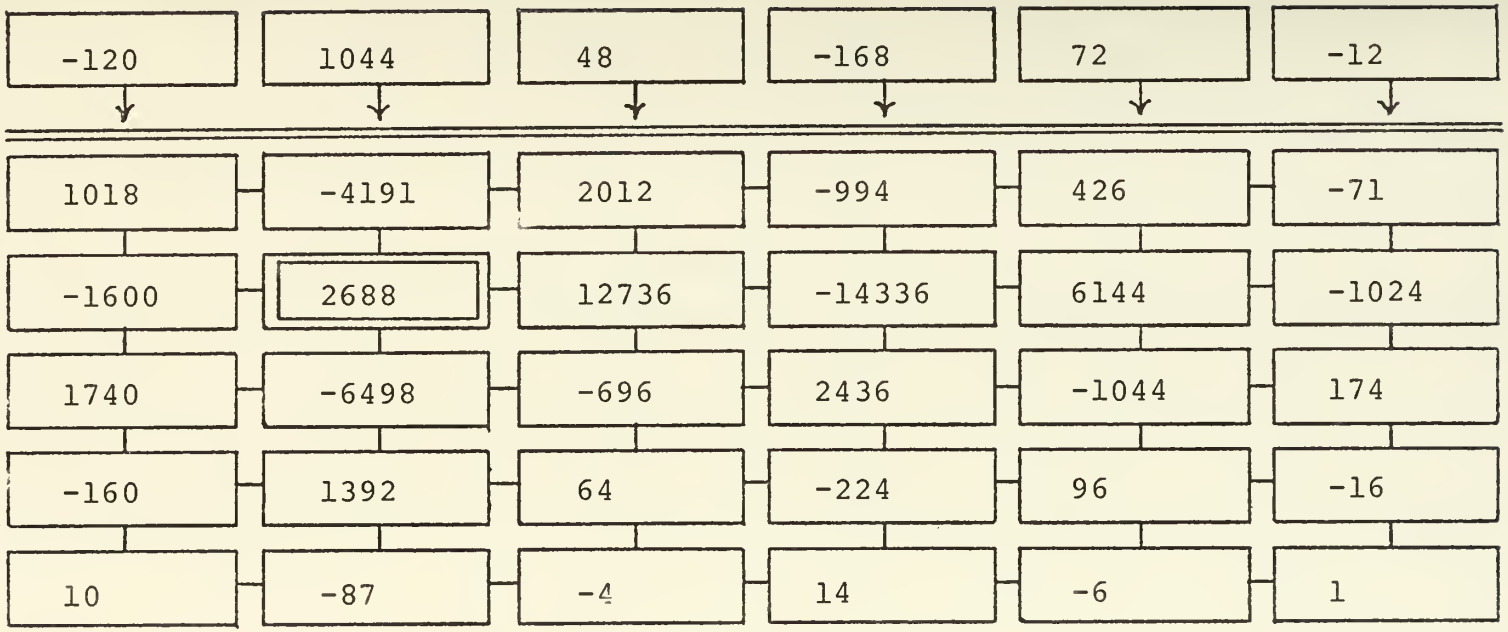
Table 3 - (Continued)



Common Factor = $\frac{1}{10{,}368h^4}$

$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial y^6}$

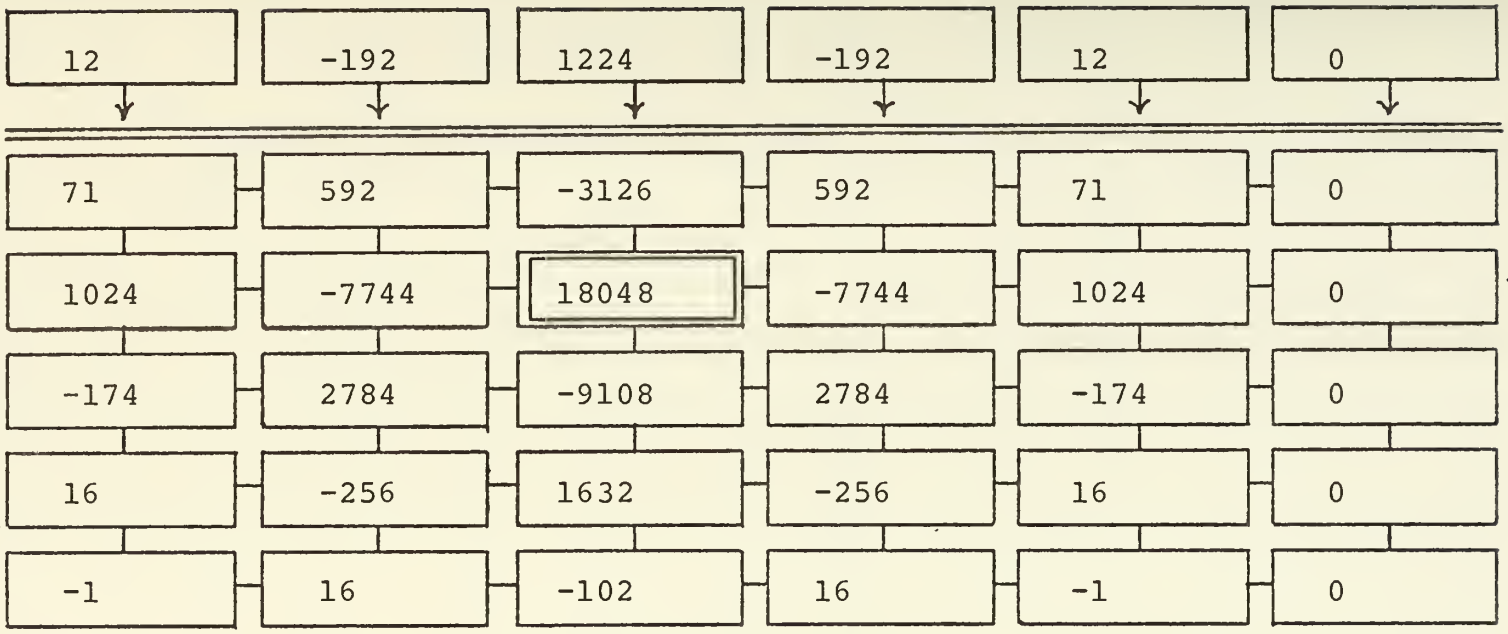
Table 3 - (Continued)



Common Factor = $\frac{1}{720h^4}$

$$E_t = + \frac{163}{150} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{2}{25} h^2 \frac{\partial^6 P}{\partial y^6}$$

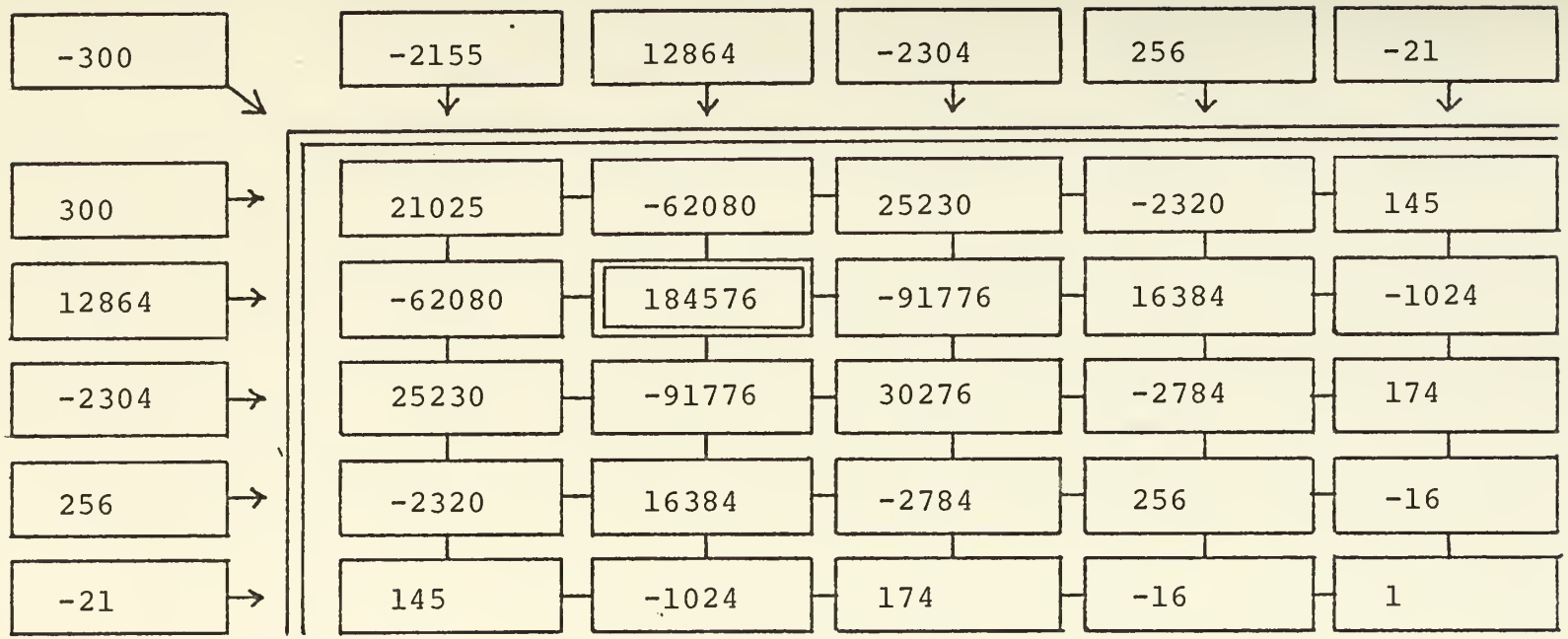
Table 4 - Finite Difference Molecules For Biharmonic Operator With Boundary Conditions Specified By the Harmonic Operator Along the Top Edge



Common Factor = $\frac{1}{720h^4}$

$$E_t = -\frac{16}{75} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{2}{25} h^2 \frac{\partial^6 P}{\partial y^6}$$

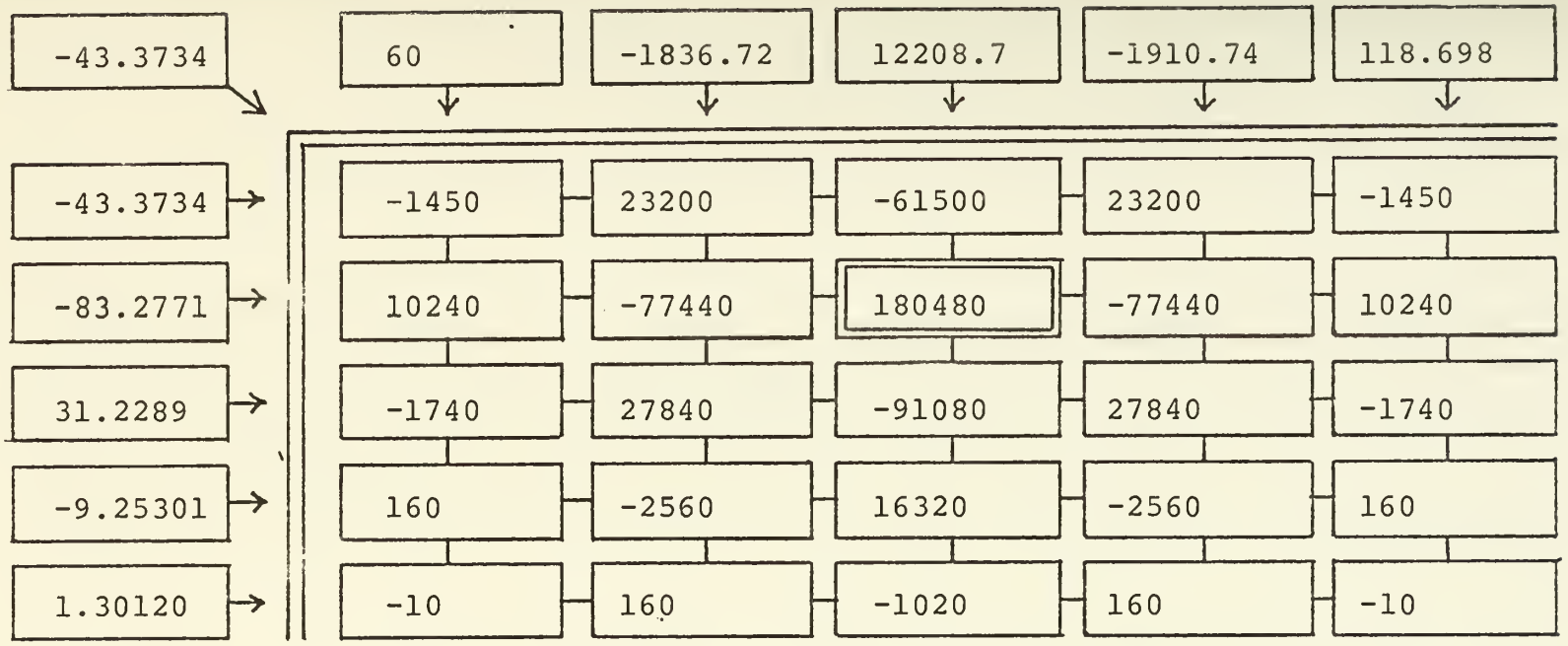
Table 4 - (Continued)



Common Factor = $\frac{1}{7200h^4}$

$$E_t = -\frac{2}{25} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{2}{25} h^2 \frac{\partial^6 P}{\partial y^6}$$

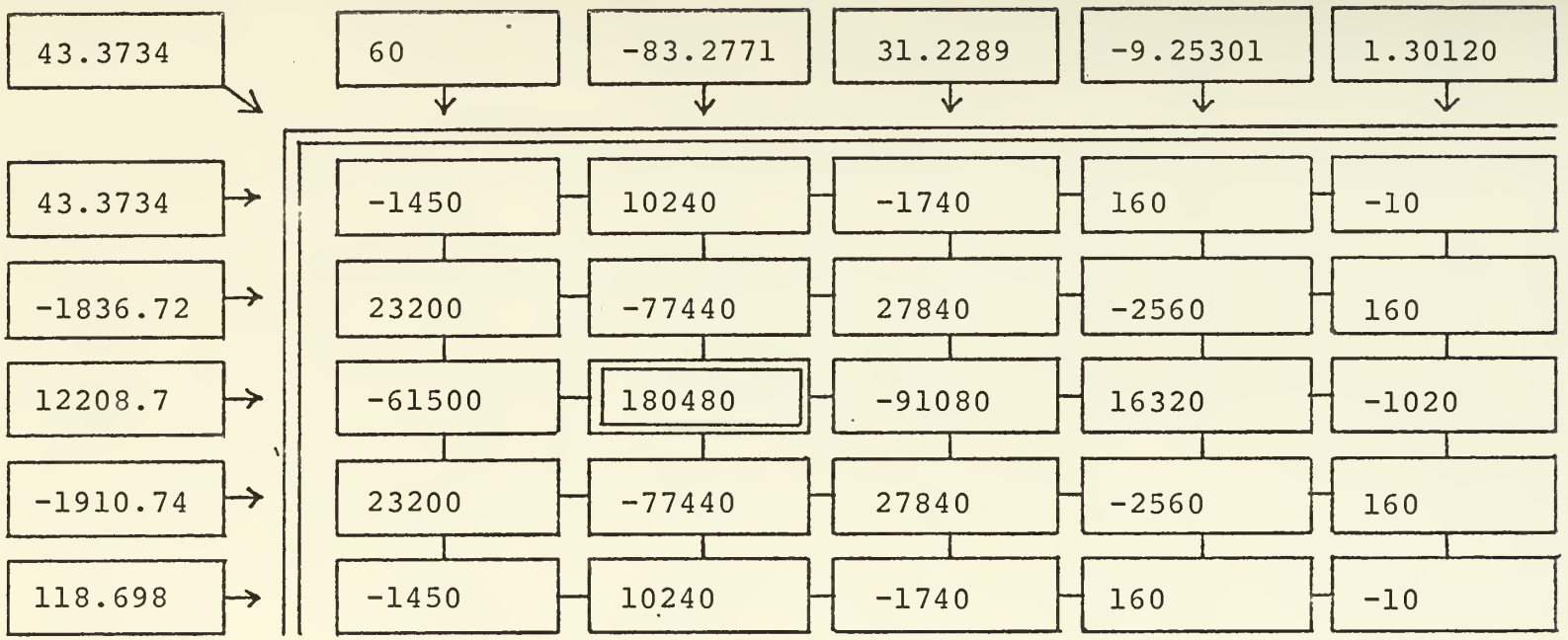
Table 5 - Finite Difference Molecule For Biharmonic Operator With Boundary Conditions of $\partial^2/\partial y^2$ Along the Top Edge and $\partial^2/\partial x^2$ Along the Left Edge



Common Factor = $\frac{1}{7200h^4}$

$$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{2}{25} h^2 \frac{\partial^6 P}{\partial y^6}$$

Table 5 - (Continued)



Common Factor = $\frac{1}{7200h^4}$

$$E_t = -\frac{2}{25} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{1}{6} h^2 \frac{\partial^6 P}{\partial y^6}$$

Table 5 - (Continued)

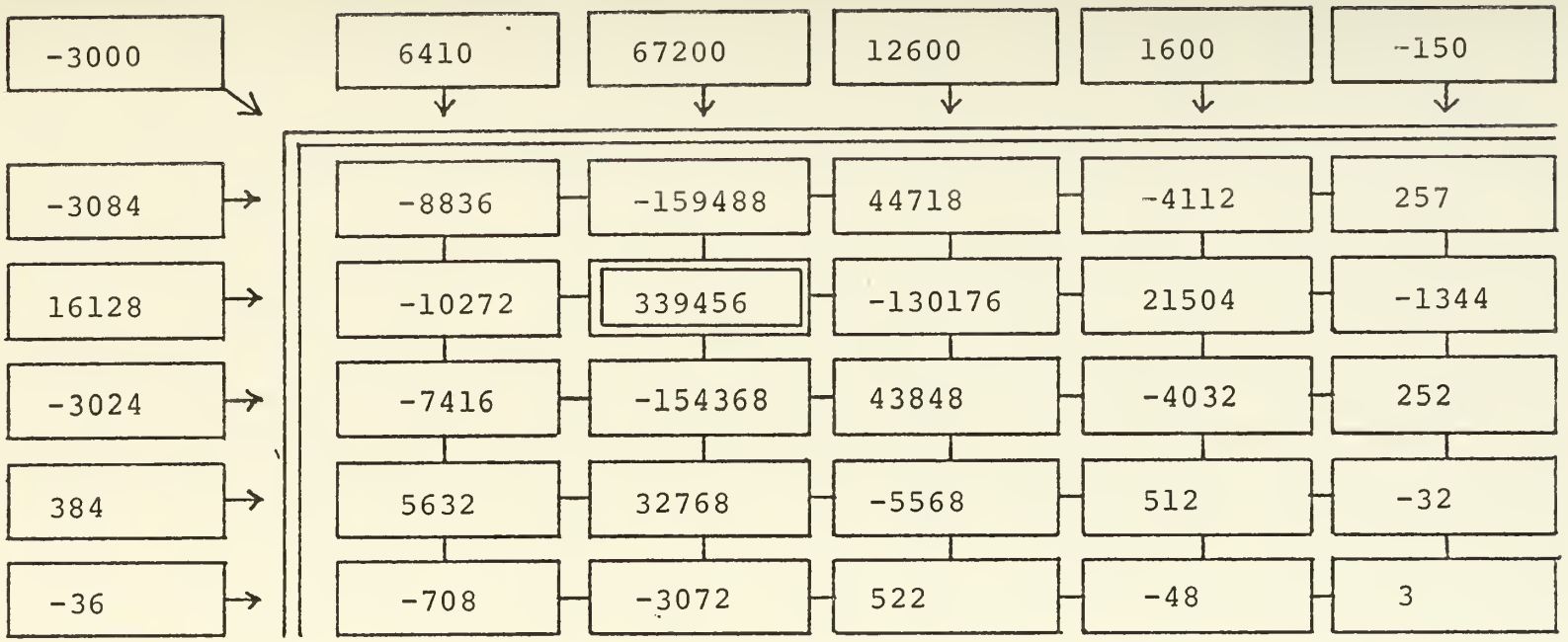
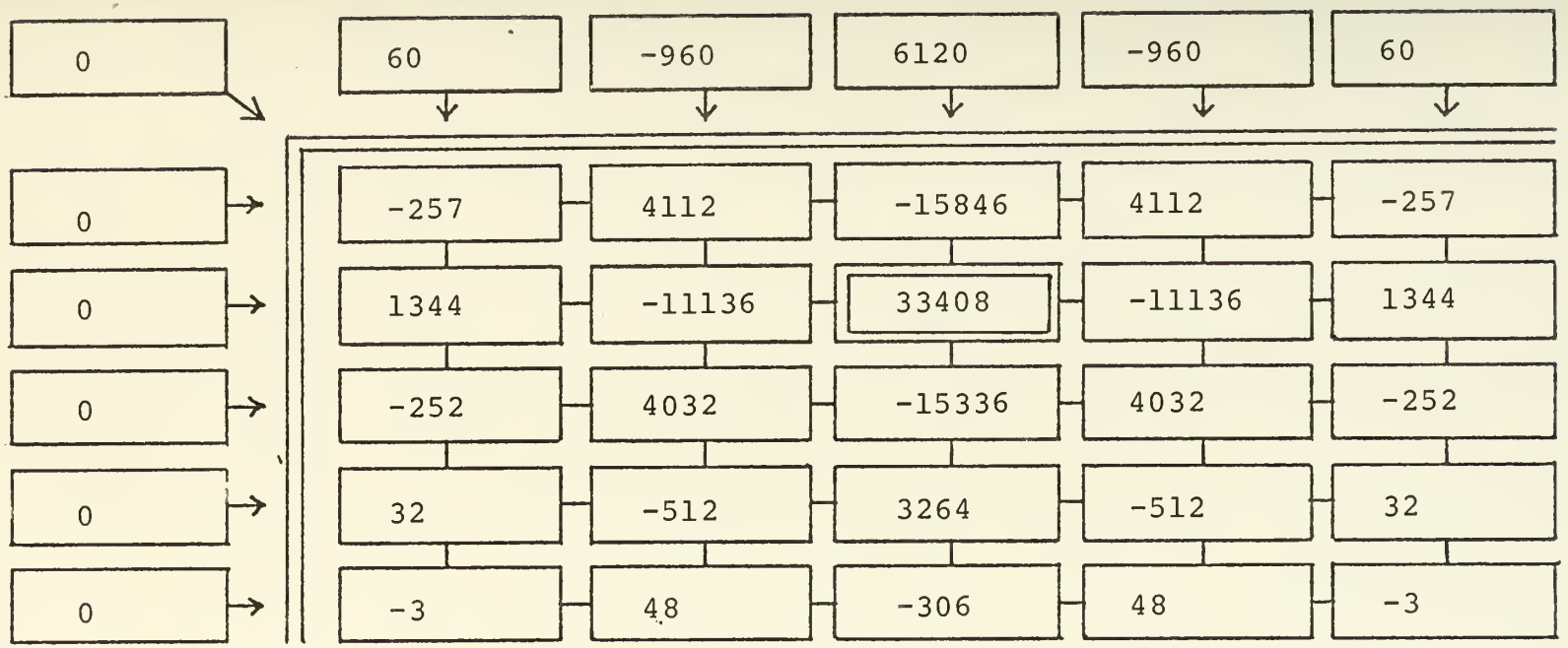


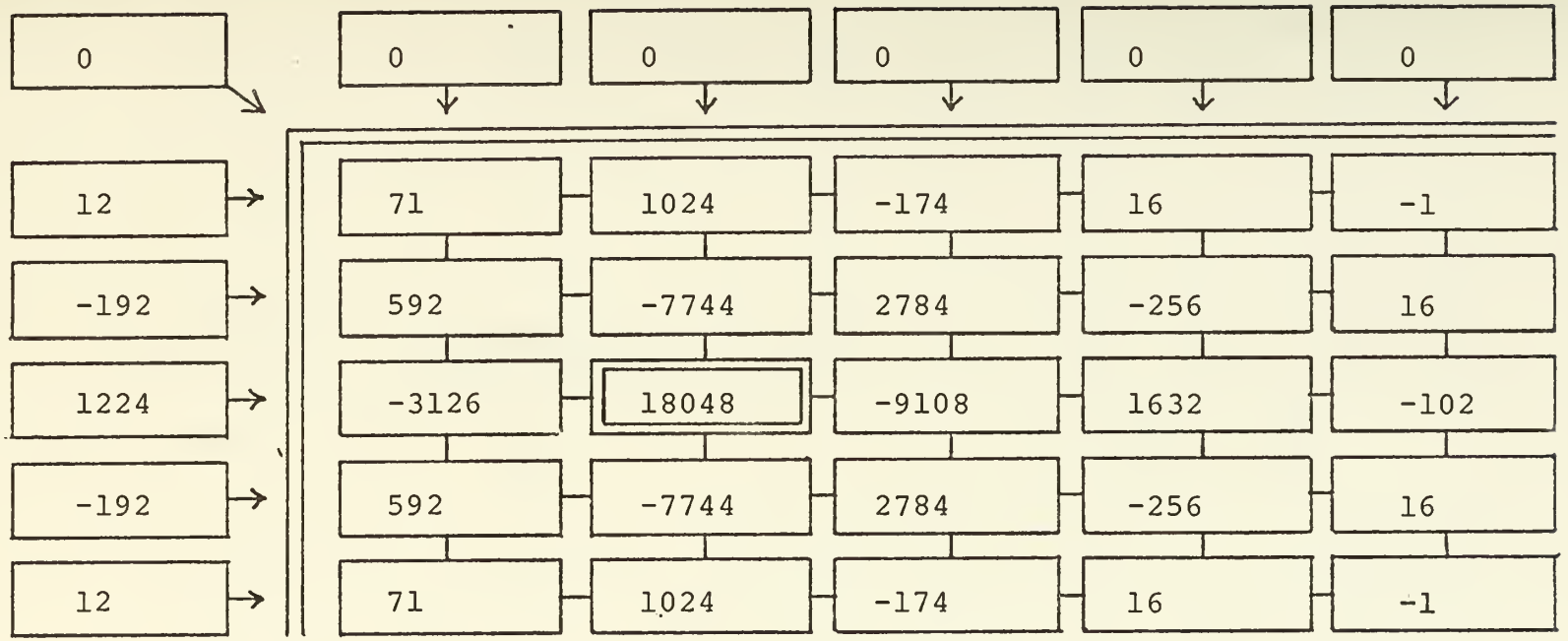
Table 6 - Finite Difference Molecule For Biharmonic Operator With Boundary Conditions Specified By the $\partial/\partial y$ Along The Top Edge And the Harmonic Operator Along The Left Edge



Common Factor = $\frac{1}{864h^4}$

$E_t = -\frac{1}{6} h^2 \frac{\partial^6 P}{\partial x^6}$

Table 6 - (Continued)



Common Factor = $\frac{1}{720h^4}$

$$E_t = -\frac{2}{25} h^2 \frac{\partial^6 P}{\partial x^6} - \frac{16}{75} h^2 \frac{\partial^6 P}{\partial y^6}$$

Table 6 - (Continued)

0	11	0	0	0
0	-56	0	0	0
0	114	0	0	0
0	-104	0	0	0
11μ	35-20μ	6μ	4μ	-μ

Common Factor = $\frac{1}{12h^2}$

$$E_t = \mathcal{O}(h^3)\left(\frac{\partial^5 P}{\partial x^5} + \frac{\partial^5 P}{\partial y^5}\right)$$

0	0	11	0	0
0	0	-56	0	0
0	0	114	0	0
0	0	-104	0	0
-μ	16μ	35-30μ	16μ	-μ

Common Factor = $\frac{1}{12h^2}$

$$E_t = \mathcal{O}(h^3)\left(\frac{\partial^5 P}{\partial x^5} + \frac{\partial^5 P}{\partial y^5}\right)$$

Table 7 - Finite Difference Molecule For $\frac{\partial^2 P}{\partial y^2} + \mu \frac{\partial^2 P}{\partial x^2}$

-33K	-216+60K	-18K	-12K	3K
176K	1008-320K	96K	64K	-16K
-396K	-1728+720K	-216K	-144K	36K
528K	1296-960K	288K	192K	-48K
-275K	-360+500K	-150K	-100K	25K

Common Factor = $\frac{1}{144h^3}$

$$E_t = \mathcal{O}(h^2)\left(\frac{\partial^5 P}{\partial x^5} + \frac{\partial^5 P}{\partial y^5}\right) \quad K = (2-\mu)$$

3K	-48K	-216+90K	-48K	3K
-16K	256K	1008-480K	256K	-16K
36K	-576K	-1728+1080K	-576K	36K
-48K	768K	1296-1440K	768K	-48K
25K	-400K	-360+750K	-400K	25K

Common Factor = $\frac{1}{144h^3}$

$$E_t = \mathcal{O}(h^2)\left(\frac{\partial^5 P}{\partial x^5} + \frac{\partial^5 P}{\partial y^5}\right) \quad K = (2-\mu)$$

Table 8 - Finite Difference Molecule For $\frac{\partial^3 P}{\partial y^3} + K\frac{\partial^3 P}{\partial x^2 \partial y}$

IV. DISCUSSION

A INTEGRITY OF DERIVED FINITE DIFFERENCE OPERATORS

Confidence in the integrity of the finite difference operators developed in this work was established by comparing the solutions for the deflection of a flat plate under uniform pressure by the finite difference method with the exact solution given by Timoshenko (Ref. 6) and Roark (Ref. 7).

Each problem studied was solved using the molecules developed in this work and general finite difference techniques. Mesh sizes of L/4, L/6, L/8, L/10, L/12, where L is the width of the square plate studied, were used in successive solutions to the problem. The solution for the maximum deflection, δ_{max}, of the plate was used as a comparison. The value obtained from successive refinement of mesh spacing for each problem was plotted versus $1/N^2$, where N is the number of divisions on one side of the plate. The resulting plots were then extrapolated to obtain the solution for a mesh having an infinite number of nodal points or the condition where the mesh spacing approaches zero. This extrapolated value is taken as the final solution for each problem and is compared with the exact solution. The above plots also indicate the convergence tendency of the solutions obtained with the molecules developed.

The first problem solved was one of a square plate under uniform pressure with all edges built-in. The problem was solved using the molecules developed in this work, (Present Method), and by means of the standard biharmonic molecule found in the literature and fictitious points, (Classical

Method). The results obtained from these methods are presented in Table (9). Figure (4) is the plot of successive solutions and illustrates the convergence trend for each method.

A brief description is given in Appendix A of the solution process for the problems studied in this work. The solution process given is the one for the Present Method.

The second problem solved was a square plate under uniform pressure with all edges simply supported. The results for the maximum deflection of the plate obtained from both methods of solution are presented in Table (10). The plot of the results is given in Figure (5).

The third problem solved was a square plate under uniform pressure with two opposite edges built-in and the other two edges simply supported. A solution using the Classical Method, although possible, was not performed. The results for the maximum deflection at the center of the plate are given in Table (11) and the convergence plot by Figure (6).

The last problem solved was a square plate under uniform pressure with two opposite edges simply supported, one edge built-in and the remaining edge free. The Classical Method is not feasible for the solution of this problem since the relationship for fictitious points outside the free edge is unknown. The use of a L/4 mesh spacing was also determined to be too coarse for a valid solution of the problem. The reason being that equations in addition to the governing equilibrium equation must be written to account for the boundary conditions

MESH SIZE SPACING	NO. OF MESH DIVISIONS	PRESENT METHOD	CLASSICAL METHOD	EXACT SOLN. REF. 6
h	N	$x10^{-3}$ PL^4/D	$x10^{-3}$ PL^4/D	$x10^{-3}$ PL^4/D
L/4	4	1.0455	1.7995	
L/6	6	1.1293	1.5343	
L/8	8	1.1813	1.4245	
L/10	10	1.2095	1.3696	
L/12	12	1.2258	1.3388	
0	∞	1.2628	1.2688	1.2637

Table 9 - Maximum Deflection of a Square Plate Built-in On All Edges Under Uniform Pressure

MESH SIZE SPACING	NO. OF MESH DIVISIONS	PRESENT METHOD	CLASSICAL METHOD	EXACT SOLN. REF. 6
h	N	$x10^{-3}$ PL^4/D	$x10^{-3}$ PL^4/D	$x10^{-3}$ PL^4/D
L/4	4	3.6555	4.0283	
L/6	6	3.8405	4.0483	
L/8	8	3.9265	4.0547	
L/10	10	3.9719	4.0575	
L/12	12	3.9979	4.0590	
0	∞	4.0570	4.0630	4.0567

Table 10 - Maximum Deflection For Square Plate Supported On All Edges Under Uniform Pressure

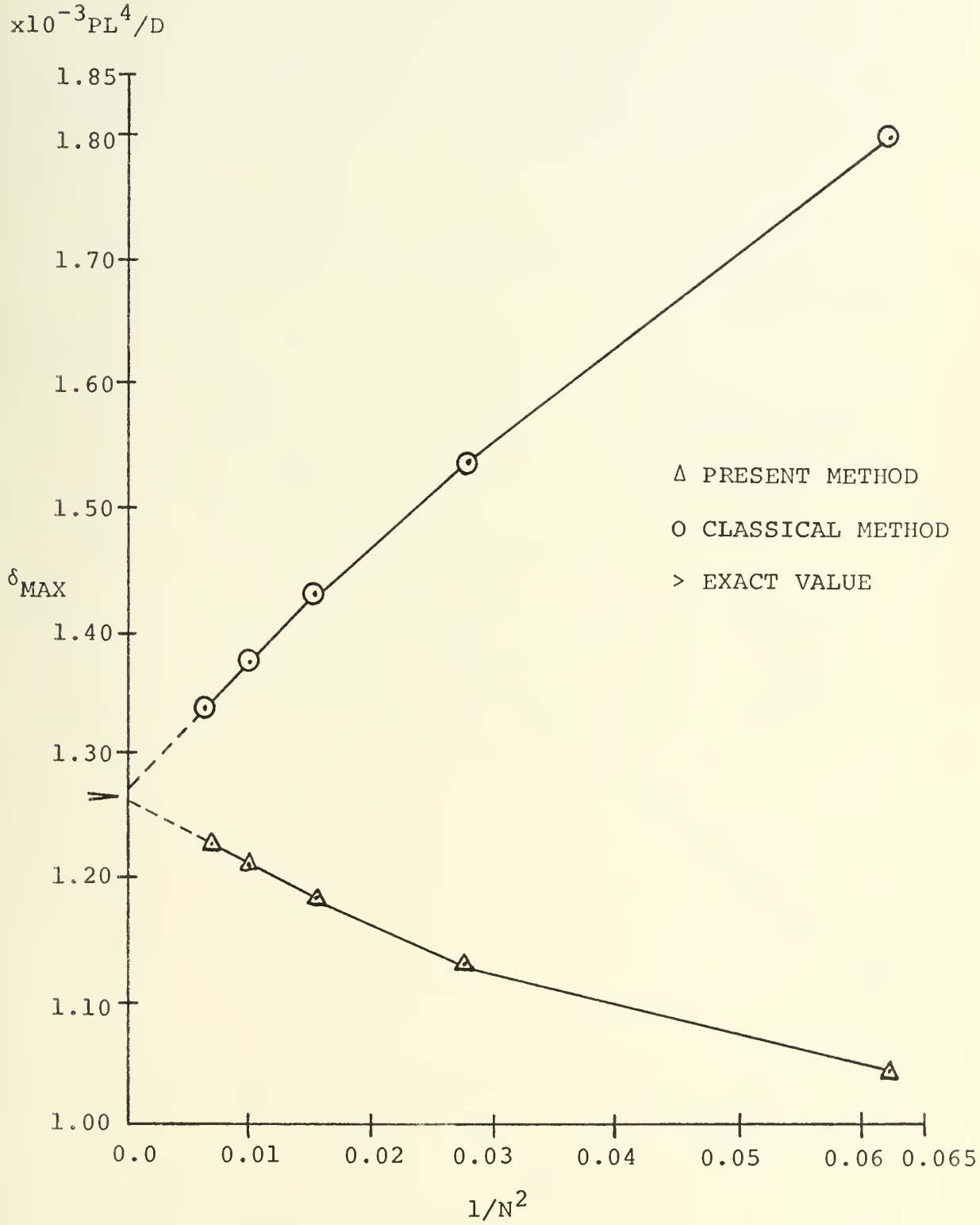


FIGURE 4 - Convergence Plot For Plate With All Edges Built-in

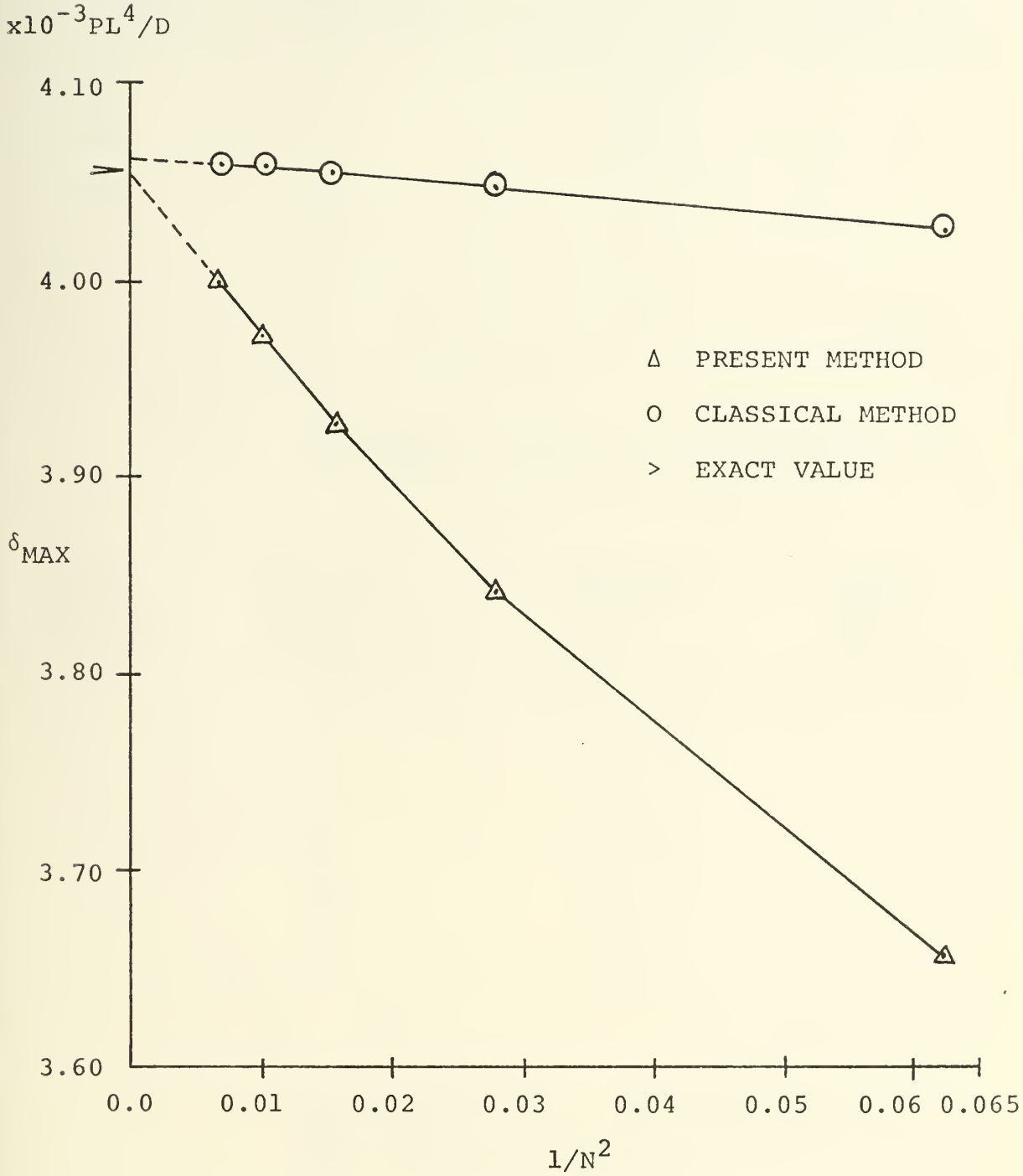


FIGURE 5 - Convergence Plot For Plate With All Edges Simply Supported

MESH SIZE SPACING	NO. OF MESH DIVISIONS	PRESENT METHOD	EXACT SOLN. REF. 7
h	N	$x10^{-3}$ PL^4/D	$x10^{-3}$ PL^4/D
L/4	4	1.6563	
L/6	6	1.7625	
L/8	8	1.8213	
L/10	10	1.8530	
0	∞	1.9094	1.9230

Table 11 - Maximum Deflection For Square Plate With Two Opposite Edges Built-in And The Other Two Simply Supported Under Uniform Pressure

MESH SIZE SPACING	NO. OF MESH DIVISIONS	PRESENT METHOD	EXACT SOLN. REF. 6
h	N	$x10^{-2}$ PL^4/D	$x10^{-2}$ PL^4/D
L/6	6	0.96672	
L/8	8	1.0017	
L/10	10	1.0320	
L/12	12	1.0533	
0	∞	1.1017	1.1263

Table 12 - Maximum Deflection For Square Plate With One Edge Built-in, One Edge Simply Supported, One Edge Free And One Edge Simply Supported Under Uniform Pressure

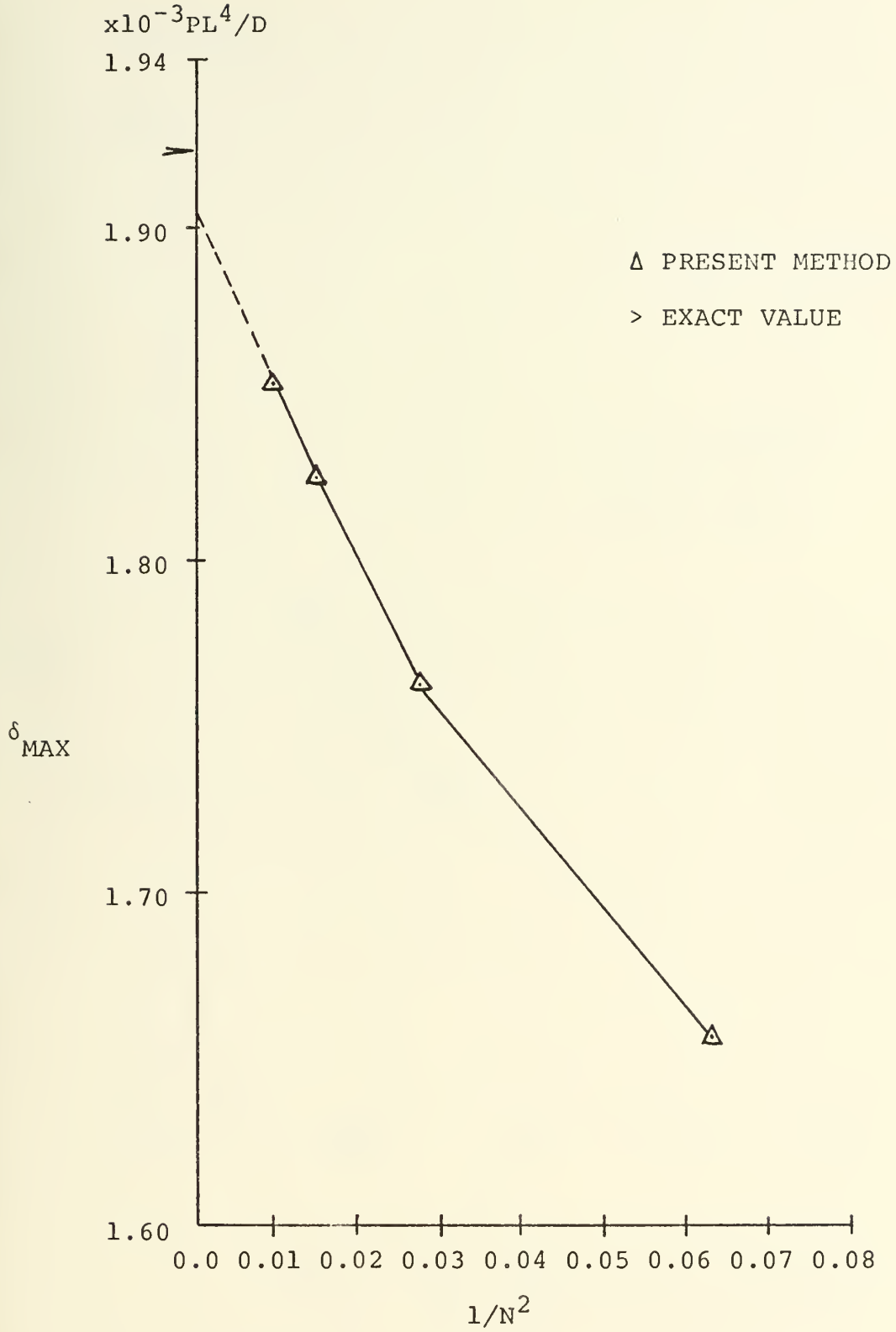


FIGURE 6 - Convergence Plot For Plate Built-in On Two Opposite Edges and Simply Supported On The Other Two Edges

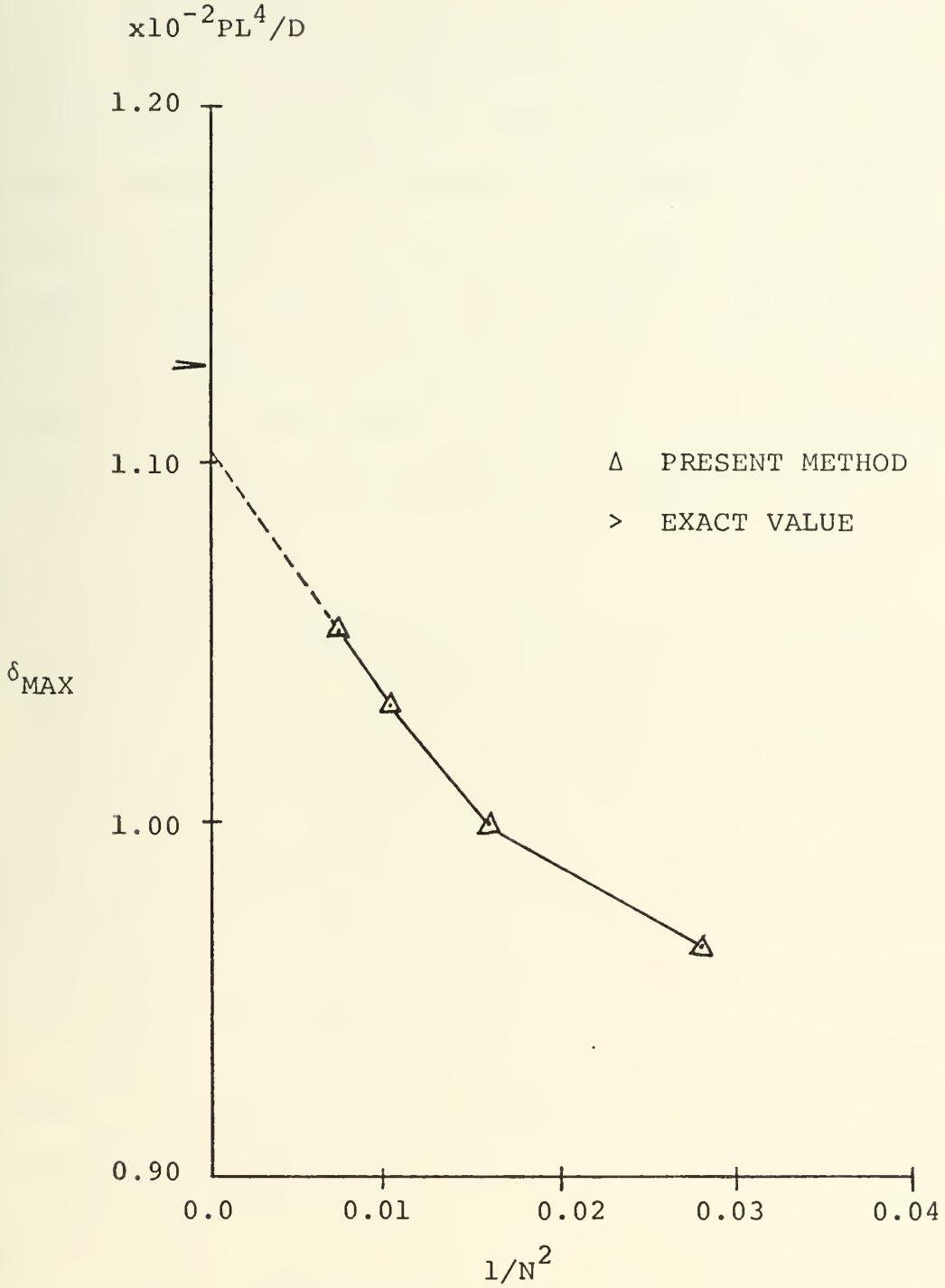


FIGURE 7 - Convergence Plot For Plat With Two Edges Simply Supported, One Edge Built-in And One Edge Free

along the free edge, since these conditions were not incorporated into the finite difference biharmonic operator. The coarse grid given by a L/4 mesh does not provide sufficient nodal points to write equations to establish complete equilibrium over the entire plate. The requirement of additional equations for this particular problem is made clearer in the solution process in Appendix A. The results for the maximum deflection of the plate are given in Table (12), and the convergence plot is illustrated by Figure (7).

B. CONCLUSIONS

Sets of mathematical molecules for the numerical approximation by finite differences of the biharmonic operator with various boundary conditions included were developed, as well as molecules for other differential operators. One consistent form of an interpolating polynomial was used to approximate the required two dimensional surface for the construction of all finite difference operators.

Solutions for various plate bending problems obtained by using the developed finite difference operators are in excellent agreement with the exact solutions found in the literature.

The convergence plots illustrate a straight convergence rate without oscillations for mesh spacings greater than L/6 for all problems where the biharmonic operator and boundary conditions may be combined into one molecule. In Figures (4)

and (5), solutions obtained by the present method are compared to the classical solutions with fictitious points. In one case the rate of convergence of the method is better than the classical method, in the other it is not. However the present method always gave a lower bound which is not always true for the classical method as shown in the two figures.

The major advantage of the molecules developed is that they may be used to solve boundary values problems without the use of fictitious nodal points. Consequently, solutions to problems such as the plate with free edge boundary condition can now be solved using finite difference operators.

One final conclusion concerning the overall aspect of the technique proposed should be made. Although the technique for developing finite difference operators proposed in this work has certain advantages over the classical method in the literature, it should be realised that other numerical methods exist for solving boundary value problems. The FINITE ELEMENT method has been applied very successfully and is covered in the literature very thoroughly, for example Refs. (8, 9 and 10).

The method of finite differences using the consistent operators developed in this work is not superior to that of finite element methods for the solution of problems that may be formulated for a finite element scheme of solution, such as plate bending problems. However, difference operators may be developed, using the technique proposed in this work, to obtain an approximate solution to any problem for which the

governing equation is known. Thus they are applicable in the solution of problems that are not easily formulated into a finite element scheme of solution.

APPENDIX A
BRIEF DESCRIPTION OF SOLUTION PROCESS

The solution of the plate bending problems by means of the finite difference operators developed in this work was performed by solving the governing equation $\nabla^4 w = p/D$ where $w = w(x,y)$ is the displacement component perpendicular to the middle plane (x,y) of the plate.

For the plate with all edges built-in, a mesh spacing of L/4 was used for the first solution. The applicable mesh is given below in Figure (8).

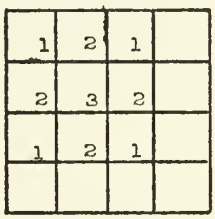


FIGURE 8 - L/4 Finite Difference Mesh For A Square Plate With All Edges Built-in Or Simply Supported

Due to symmetry and the fact that w=0 along the boundaries, there are only three unknown values of deflections as shown in Figure (8). For each unknown nodal deflection, the governing equation for plate equilibrium is written with the biharmonic operator being approximated by the appropriate difference operator developed in this work. The resulting set of simultaneous equations are then solved for the unknown deflections. For this problem the following molecules were used to express the governing equation

1. Molecule from Table (3) for co-ordinate (1,3) applied at nodal point one.
2. Molecule from Table (3) for co-ordinate (2,3) applied at nodal point two.
3. Molecule from Table (1) applied at nodal point three.

The derivatives required for the nodal points along the boundaries are set to zero, thus establishing zero slope along the built-in edges.

For the plate with all edges simply supported, the same mesh (Fig. (8)) is applicable for the first finite difference solution.

The three unknown deflections are determined in this case by evaluating the governing equation with the following molecules

1. Molecule from Table (5) for co-ordinate (1,3) applied at nodal point one.
2. Molecule from Table (5) for co-ordinate (2,3) applied at nodal point two.
3. Molecule from Table (1) applied at nodal point three.

The derivatives required for the nodal points along the boundaries are set to zero, establishing zero moment for the simply supported restraints.

For a plate with two opposite edges built-in and two edges simply supported, the L/4 mesh shown in Fig. (9) is applicable

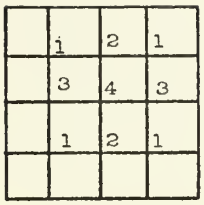


FIGURE 9 - L/4 Finite Difference Mesh For A Square Plate With Top And Bottom Edges Built-in And Side Edges Simply Supported

In this case, after applying symmetry and the fact of zero deflection along the edges, there are four unknowns to be determined. The required equations are written using the following molecules

1. Molecule from Table (6) for co-ordinate (1,3) applied at nodal point one.
2. Molecule from Table (6) for co-ordinate (2,3) applied at nodal point two.
3. Molecule from Table (6) for co-ordinate (1,2) applied at nodal point three.
4. Molecule from Table (1) applied at nodal point four.

As before, the values of the derivatives specified by the boundary conditions are set to zero.

For the plate with built-in, simply supported, free and simply supported edges, a mesh spacing of L/6 was used for the first finite difference solution as shown in Fig. (10).

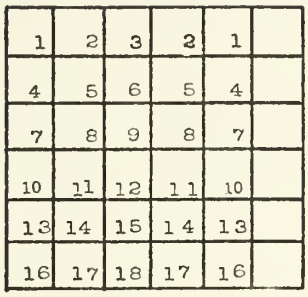


FIGURE 10 - L/6 Finite Difference Mesh For A Square Plate With Top Edge Built-in, Sides Simply Supported, And Bottom Edge Free

After applying symmetry and the fact that the deflection is zero on all boundaries except the free one, eighteen unknown deflections remain in the L/6 mesh. These unknowns are determined by solving the governing equation for nodal points 1 through 12 and the boundary condition equations of shear and moment along a free edge for nodal points 16, 17, and 18. This requirement of using the nodal points along the free edge to specify the applicable boundary conditions at this location reduces the number of nodal points for which the governing equilibrium equation may be written. Consequently, an L/4 grid spacing was found to be too coarse for a valid solution of the problem.

The required eighteen equations are written using the following finite difference molecules;

1. Molecule from Table (6) for co-ordinate (1, 3) applied at nodal point one.
2. Molecule from Table (6) for co-ordinate (2, 3) applied at nodal point two.
3. Molecule from Table (2) for co-ordinate (2, 3) applied at nodal point three.

4.	Molecule from Table (6) for co-ordinate (1, 2) applied at nodal point four.
5,6,8, 9,11, 12.	Molecule from Table (1) applied at nodal points 5,6,8,9,11, and 12.
7,10.	Molecule from Table (4) for co-ordinate (2, 3) applied at nodal points seven and ten. In this case, the molecule is laid on the finite difference mesh in the y direction so that the specified boundary condition constructed in the operator is along the simply supported edge.
13.	Molecule from Table (7) for co-ordinate (1, 0) is applied at nodal point sixteen.
14,15.	Molecule from Table (7) for co-ordinate (2, 0) is applied at nodal points seventeen and eighteen.
16.	Molecule from Table (8) for co-ordinate (1, 0) is applied at nodal point sixteen.
17,18.	Molecule from Table (8) for co-ordinate (2, 0) is applied at nodal points seventeen and eighteen.

Values for the derivatives along the built-in and simply supported edges required in the solution of this problem are set to zero to account for the specified boundary conditions.

In order to obtain sufficient values for the deflection at a particular nodal point for the construction of a convergence plot, successive solutions are performed using a refinement in the mesh spacing for each solution.

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13. ABSTRACT

A new technique for constructing "computational molecules" for linear finite difference operators is developed. The basic approach is one of approximating a two dimensional surface with a geometrically consistent interpolating polynomial of degree four or five. The desired finite difference operator is then developed from the polynomial. The resulting molecules are geometrically consistent and may be used to solve boundary value problems without the use of fictitious points.

Molecules for the biharmonic operator with various boundary conditions included are presented int his paper, as well as molecules representing the boundary conditions for shear and moment along the free edge of a plate.

The integrity of the molecules presented is proven by comparison of solutions for flat plate bending problems by finite difference with exact solutions from the literature. Convergence plots for each problem are also presented.

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